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Computational AGility for internal flows simulations and comparisons with Experiments

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

IN PARTNERSHIP WITH:
CNRS
Université de Pau et des Pays de l’Adour

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations
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2. Overall Objectives

2.1. Turbulent flows with complex interactions

This interdisciplinary project brings together researchers coming from different horizons and backgrounds (applied mathematics and fluid mechanics) who progressively elaborated a common vision of what should be the simulation tool of fluid dynamics of tomorrow. Our application will be focused on wall bounded turbulent flows and featuring complex phenomena such as aeroacoustics, hydrodynamic instabilities, phase change processes, complex walls, buoyancy or localized relaminarization. Because such flows are exhibiting a multiplicity of time and scale fluctuations resulting from complex interactions, their simulation is extremely challenging. Even if various methods of simulation (DNS $^0$, RANS $^0$, LES $^0$, hybrid RANS-LES) are available and have been significantly improved over time, none of them does satisfy all the needs encountered in industrial and environmental configurations. We consider that all these methods will be useful in the future in different situations or regions of the flow if combined in the same simulation in order to benefit from their respective advantages wherever relevant, while mutually compensating their known limitations. It will thus lead to a description of turbulence at widely varying scales in the computational domain, hence the name **multi-scale simulations**. For example, the RANS mode may extend throughout regions where turbulence is sufficiently close to equilibrium leaving to LES or DNS the handling of regions where large scale coherent structures are present. However, a considerable body of work is required to:

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$^0$Direct numerical simulation

$^0$Reynolds averaged Navier-Stokes

$^0$Large-eddy simulation
• Establish the behavior of the different types of turbulence modeling approaches when combined with high order discretization methods.
• Elaborate relevant and robust switching criteria between models, similar to error assessments used in automatic mesh refinement, but based on the physics of the flow in order to adapt on the fly the scale of resolution from one extreme of the spectrum to another (say from the Kolmogorov scale to the geometrical large scale, i.e., from DNS to RANS).
• Ensure a high level of accuracy and robustness of the resulting simulation tool to address a large range of flow configurations, i.e., from a generic lab scale geometry for validation to practical systems of interest of our industrial partners.

But the best agile modeling and high order discretization methods are useless without the recourse to high performance computing (HPC) to bring the simulation time down to values compatible with the requirement of the end users. So, a significant part of our activity will be devoted to the proper handling of the constantly evolving supercomputer architectures. But even the best ever simulation library is useless if it is not disseminated and increasingly used by the CFD community as well as our industrial partners. In that respect, the significant success of the low order finite volume simulation suite OpenFOAM \(^0\) or the more recently proposed SU2 \(^0\) from Stanford are considered as examples of quite successful dissemination stories that could be if not followed but at least considered as a source of inspiration. Our natural inclination though will be to promote the use of the library in direction of our present and future industrial and academic partners with a special interest on the SMEs active in the highly competitive and strategic economical sectors of energy production and aerospace propulsion. Indeed, these sectors are experiencing a revolution of the entire design process especially for complex parts with an intimate mix between simulations and additive manufacturing (3D printing) processes in the early stages of the design process. For big companies such as General Electric or Safran (co-developing the CFM Leap-1 engines with 3D printed fuel nozzles) as well as medium-size companies such as Aerojet Rocketdyne, this is a unique opportunity to reduce the duration and hence the cost of development of their systems while preserving if not strengthening their capability of designing innovative components that cannot be produced by classical manufacturing processes. On the other side, for the small companies of this sector, this may have a rather detrimental effect on their competitiveness since their capability of mastering both these new manufacturing processes and advanced simulation approaches is far more limited. Thus, through our sustained direct (EDF, Turbomeca, PSA, AD Industrie) or indirect (European programs, WALLTURB, KIAI, IMPACT-AE, SOPRANO) partnership with different companies, we are able to identify relevant generic configurations from our point of view of scientists to serve as support for the development of our approach. This methodological choice was motivated by the desire to lead an as efficient as possible transfer activity while maintaining a clear distinction between what falls within our field of competence of researchers from what is related to the development of their products by our industrial partners.

The long-term objective of this project is to develop, validate, promote and transfer an original and effective approach for modeling and simulating generic flows representative of flow configurations encountered in the field of energy production and aeronautical propulsion. Our approach will be combining mesh (h) + turbulence model (m) + discretization order (p) agility. This will be achieved by:

• Contributing to the development of new turbulence models.
• Improving high order numerical methods, and increasing their efficiency in the constantly evolving High Performance Computing context.
• Developing experimental tools.

Concerning applications, our objective are:

• To reinforce the long term existing partnership with EDF and Safran group, and the other European partners involved in the same European projects as we are.
• To consolidate and develop partnership with SMEs operating in the aeronautical sector.

\(^0\)http://www.openfoam.com
\(^0\)http://su2.stanford.edu/
3. Research Program

3.1. The scientific context

3.1.1. Computational fluid mechanics: modeling or not before discretizing?

A typical continuous solution of the Navier-Stokes equations at sufficiently high values of the Reynolds number is governed by a spectrum of time and space scales fluctuations closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [32] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to $Re$ per dimension. The smallest scales play a crucial role in the dynamics of the largest ones which implies that an accurate framework for the computation of turbulent flows must take into account all these scales. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step followed by the simulation runs themselves. If a modeling phase is on the agenda, then one has to choose again among the above mentioned variety of approaches. As it is illustrated in Fig. 1, this can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying a statistical averaging (RANS) or a spatial filtering operator to the Navier-Stokes equations (LES). The new terms brought about by the filtering operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones supposed to be more isotropic, LES proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was progressively applied to geometries of increasing complexity (channel flows with values of $Re_{τ}$ multiplied by 10 during the last 15 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool that permits (i) to improve our knowledge on turbulent flows and (ii) to test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, the high computational cost of LES or DNS makes necessary the use of highly accurate numerical schemes in order to optimize the use of computational resources. To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program 0, once chosen, a single turbulence model will (try to) do the job for modeling the whole flow. Thus, depending on its intrinsic strengths and weaknesses, the accuracy will be a rather volatile quantity strongly dependent on the flow configuration. The turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the deficiencies of both approaches and to combine them for significantly improving the overall quality of the modeling, the hybrid RANS-LES approach has emerged during the last decade as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, connected with a time filtered hybrid RANS-LES and a systematic and progressive validation process against experimental data produced by the team.

0https://cordis.europa.eu/result/rcn/177053_en.html
Figure 1. A schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate of increase in computer performances).

3.1.2. Computational fluid mechanics: high order discretization on unstructured meshes and efficient methods of solution

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [43] and first studied by Lesaint and Raviart [39]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high order ENO schemes, whereas specific constraints given by the finite element nature of the scheme were progressively solved, for scalar conservation laws [28], [27], one dimensional systems [26], multidimensional scalar conservation laws [25], and multidimensional systems [29]. For the same system, we can also cite the work of [31], [36], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. Contrary to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [18]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [23] by mean of a mixed formulation. Actually, this first attempt led to a non compact computation stencil, and was later proved to be not stable. A compactness improvement was made in [24], which was later analyzed, and proved to be stable in a more unified framework [19]. The combination with the $k - \omega$ RANS model was made in [22]. As far as Navier Stokes equations are concerned, we can also cite the work of [34], in which the stabilization is closer to the one of [19], the work of [40] on local time stepping, or the first use of discontinuous Galerkin methods.
for direct numerical simulation of a turbulent channel flow done in [30]. Discontinuous Galerkin methods are so popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high order finite volumes, which require as more and more neighbors as the order increases.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [21]. This is a pro compared not only with finite differences schemes, which can be developed only on structured meshes, but also compared with continuous finite elements methods, for which the definition of the approximation basis is not clear on aggregated elements.
- $p$-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

For concluding this section, there already exist numerical schemes based on the discontinuous Galerkin method which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain many things to be improved, which include: efficient shock capturing methods for supersonic flows, high order discretization of curved boundaries, low Mach number behavior of these schemes and combination with second-moment RANS models. Another drawback of the discontinuous Galerkin methods is that they can be computationally costly, due to the accurate representation of the solution calling for a particular care of implementation for being efficient. We believe that this cost can be balanced by the strong memory locality of the method, which is an asset for porting on emerging many-core architectures.

### 3.1.3. Experimental fluid mechanics: a relevant tool for physical modeling and simulation development

With the considerable and constant development of computer performance, many people were thinking at the turn of the 21st century that in the short term, CFD would replace experiments considered as too costly and not flexible enough. Simply flipping through scientific journals such as Journal of Fluid Mechanics, Combustion of Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac is sufficient to convince oneself that the recourse to experiments to provide either a quantitative description of complex phenomena or reference values for the assessment of the predictive capabilities of the physical modeling and of the related simulations is still necessary. The major change that can be noted though concerns the content of the interaction between experiments and CFD (understood in the broad sense). Indeed, LES or DNS assessment calls for the experimental determination of time and space turbulent scales as well as time resolved measurements and determination of single or multi-point statistical properties of the velocity field. Thus, the team methodology incorporates from the very beginning an experimental component that is operated in strong interaction with the physical modeling and the simulation activities.

### 3.2. Research directions

#### 3.2.1. Boundary conditions

##### 3.2.1.1. Generating synthetic turbulence

A crucial point for any multi-scale simulation able to locally switch (in space or time) from a coarse level of turbulence description to a more refined one, is the enrichment of the solution by fluctuations as physically meaningful as possible. Basically, this issue is an extension of the problem of the generation of realistic inlet boundary conditions in DNS or LES of subsonic turbulent flows. In that respect, the method of anisotropic

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0 http://www.ercoftac.org
linear forcing (ALF) we have developed in collaboration with EDF proved very encouraging, by its efficiency, its generality and simplicity of implementation. So, it seems natural, on the one hand, to extend this approach to the compressible framework and then implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou in the framework of a just-started CIFRE PhD) on the theoretical link between the local variations of the scale’s description of turbulence (e.g. a sudden variations in the size of the time filter) and the intensity of the ALF forcing transiently applied to help in the development of missing scales of fluctuations.

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A lot of work has already been done for second order schemes for Navier Stokes equations, see [42], [45] and the huge number of papers citing it. On the one hand, we believe that strong improvements are necessary with higher order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this, we will first concentrate on the linearized Navier-Stokes system, and analyze the boundary condition imposition in a discontinuous Galerkin framework with a similar approach as in [33]. We will also try to extend the work of [46], which deals with Euler equations, to the Navier Stokes equations.

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero Mach models to the compressible system

We shall develop in parallel our multi-scale turbulence modeling and the related adaptive numerical methods of AeroSol. Without prejudice to methods that will be on the podium in the future, a first step in this direction will be to extend to a compressible framework the continuous hybrid temporal RANS/LES models we have developed up to now in a Mach zero context.

3.2.2.2. Study of wall flows with and without mass or heat transfer at the wall: determination and validation of relevant criteria for hybrid turbulence models

In the targeted application domains, the turbulence/wall interaction and the heat transfer at the fluid-solid interfaces are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfers. For our part, we will gradually use all our analysis and experimentation tools to actively participate in the improvement of the collective knowledge on such kind of transfers. The flow configurations dealt with by the beginning of the project will be those of subsonic single phase impacting jets or JICF with the possible presence of an interacting acoustic wave. The conjugate heat transfer at the wall will be also progressively tackled. The existing criteria of switching of the hybrid RANS/LES model will be tested on those flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine if it is possible to drive a change of instability regime (e.g. from absolute to convective) and so propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES one.

3.2.2.3. Improvement of turbulence models

The production and the subsequent use of DNS (AeroSol library) and experimental (bench MAVERIC) databases dedicated to the improvement of the physical models will be an important part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. It is on the improvement of the hybrid RANS/LES approach that will focus most of our initial efforts of analysis of the DNS and experimental data as soon as they will become available. This method has a decisive advantage over all other hybrid RANS/LES approaches since it relies on a well defined time filtering formalism. This greatly facilitates the proper extraction from the databases of the various terms appearing in the relevant flux balances obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central
issue will also be to answer positively the following question: will we be comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

3.2.3. Development of an efficient implicit high-order compressible solver scalable on new architectures

As the flows we wish to simulate may be very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

- Efficient implementation of the discontinuous Galerkin method.
- Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid.
- Porting on heterogeneous architectures.
- Implementation of models.

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

In high order discontinuous Galerkin methods, the unknown vector is composed of a concatenation of the unknowns in the cells of the mesh. An explicit residual computation is composed of three loops: an integration loop on the cells, for which computations in two different cells are independent, an integration loop on boundary faces, in which computations depend on data of one cell and on the boundary conditions, and an integration loop on the interior faces, in which computations depend on data of the two neighboring cells. Each of these loops is composed of three steps: the first step consists in interpolating data at the quadrature points, the second step in computing a nonlinear flux at the quadrature points (the physical flux for the cell loop, an upwind flux for interior faces or a flux adapted to the kind of boundary condition for boundary faces), and the third step consists in projecting the nonlinear flux on the degrees of freedom.

In this research direction, we propose to exploit the strong memory locality of the method (i.e., the fact that all the unknowns of a cell are stocked contiguously). This formulation can reduce the linear steps of the method (interpolation on the quadrature points and projection on the degrees of freedom) to simple matrix-matrix product which can be optimized. For the nonlinear steps, composed of the computation of the physical flux on the cells and of the numerical flux on the faces, we will try to exploit vectorization.

3.2.3.2. Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid

For our computations of the IMPACT-AE project, we use an explicit time stepping. The time stepping is limited by the CFL condition, and in our flow, the time step is limited by the acoustic wave velocity. As the Mach number of the flow we simulate in IMPACT-AE is low, the acoustic time restriction is much lower than the turbulent time scale, which is driven by the velocity of the flow. We hope to have a better efficiency by using time implicit methods, for using a time step driven by the velocity of the flow.

Using implicit time stepping in compressible flows is particularly difficult, because the system is fully nonlinear, so that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high order framework, because the optimization of the memory usage is very difficult. That is why we propose to use Jacobian free implementation, based on [38]. This method consists in solving the linear steps of the Newton method by a Krylov method, which requires Jacobian-vector product. The smart idea of this method is to replace this product by an approximation based on a difference of residual, therefore avoiding any Jacobian computation. Nevertheless, Krylov methods are known to converge slowly, especially for the compressible system when the Mach number is low, because the system is ill-conditioned. In order to precondition, we propose to use an aggregation-based multigrid method, which consists in using the same numerical method on coarser meshes obtained by aggregation of the initial mesh. This choice is driven by the fact that multigrid methods are the only one to scale linearly [47], [48] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.
Beyond the technical aspects of the multigrid approach, which will be challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) \cite{41}. For this, we propose to extend the scalar analysis of \cite{49} to a linearized version of the Euler and Navier-Stokes equations, and try to deduce an optimal strategy for anisotropic aggregation, based on the local characteristics of the flow. Note that discontinuous Galerkin methods are particularly well suited to h-p aggregation, as this kind of methods can be defined on any shape \cite{21}.

3.2.3.3. Porting on heterogeneous architectures

Until the beginning of the 2000s, the computing capacities have been improved by interconnecting an increasing number of more and more powerful computing nodes. The computing capacity of each node was increased by improving the clock speed, the number of cores per processor, the introduction of a separate and dedicated memory bus per processor, but also the instruction level parallelism, and the size of the memory cache. Even if the number of transistors kept on growing up, the clock speed improvement has flattened since the mid 2000s \cite{44}. Already in 2003, \cite{35} pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. In this task, we will work on the heterogeneous aspects of computation. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a local structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU \cite{37}, as only straight simplicial cell shapes were addressed. For managing at best our heterogeneous computations on heterogeneous architectures, we propose to use the execution runtime StarPU \cite{20}. For this, the discontinuous Galerkin algorithm will be reformulated in term of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one task of the project will consist in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks will be discussed.

Last, we point out that the combination of shared-memory and distributed-memory parallel programming models is better suited than only the distributed-memory one for multigrid, because in a hybrid version, a wider part of the mesh shares the same memory, therefore allowing for a coarser aggregation.

The consortium will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high performance computing, which is one of the strategic axis of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, thanks to its formalism of temporal filtering, the HTLES approach offers a theoretical framework characterized by a continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its configuration complexity. The
first step in this direction was taken in 2017 during the internship of Axelle Perraud, who has implemented a turbulence model ($k$-$\omega$-SST) in the Aerosol library.

3.2.4. Validation of the simulations: test flow configurations

To supplement whenever necessary the test flow configuration of MAVERIC and apart from configurations that could emerge in the course of the project, the following configurations for which either experimental data, simulation data or both have been published will be used whenever relevant for benchmarking the quality of our agile computations:

- The impinging turbulent jet (simulations).
- The ORACLES two-channel dump combustor developed in the European projects LES4LPP and MOLECULES.
- The non reactive single-phase PRECCINSTA burner (monophasic swirl), a configuration that has been extensively calculated in particular with the AVBP and Yales2 codes.
- The LEMCOTEC configuration (monophasic swirl + effusion cooling).
- The ONERA MERCATO two-phase injector configuration provided the question of confidentiality of the data is not an obstacle.
- Rotating turbulent flows with wall interaction and heat transfer.
- Turbulent flows with buoyancy.

4. Application Domains

4.1. Aeroengines

Cagire is presently involved in studies mainly related with two subcomponents of the combustion chamber of aeroengines:

- The combustion chamber wall: the modelling, the simulation and the experimentation of the flow around a multiperforated plate representative of a real combustion chamber wall are the three axes we have been developing during the recent period. The continuous improvement of our in-house test facility Maveric is also an important ingredient to produce our own experimental validation data for isothermal flows. For non-isothermal flows, our participation in the EU funded program Soprano will be giving us access to non-isothermal data produced by Onera.
- The fuel nozzle: the impact of small geometrical variations related to the fabrication process on the pressure losses of the injector is being studied for a generic geometry provided by our industrial partner AD Industrie. RANS based simulations are intended to help designing some critical components of the fuel nozzle. A project is currently written to answer a call of the Nouvelle Aquitaine region, with the objective of extending this study to hybrid RANS/LES methods.

4.2. Power stations

R. Manceau has established a long term collaboration (4 CIFRE PhD theses in the past, 2 ongoing) with the R & D center of EDF of Chatou, for the development of refined turbulence models in the in-house CFD code of EDF, Code_Saturne:

- The prediction of heat transfer in fluid and solid components is of major importance in power stations, in particular, nuclear power plants. Either for the thermohydraulics of the plenum or in the study of accidental scenarios, among others, the accurate estimation of wall heat transfer, mean temperatures and temperature fluctuations are necessary for the evaluation of relevant thermal and mechanical design criteria. The PhD thesis (CIFRE EDF) of G. Mangeon is dedicated to the development of relevant RANS models for these industrial applications.
Moreover, the prediction of unsteady hydrodynamic loadings is a key point for operating and for safety studies of PWR power plants. Currently, the static loading is correctly predicted by RANS computations but when the flow is transient (as, for instance, in Reactor Coolant Pumps, due to rotor/stator interactions, or during operating transients) or in the presence of large, energetic, coherent structures in the external flow region, the RANS approach is not sufficient, whereas LES is still too costly for a wide use in industry. This issue constitutes the starting point of the just-started PhD thesis (CIFRE EDF) of Vladimir Duffal.

4.3. Automotive propulsion

The engine (underhood) compartment is a key component of vehicle design, in which the temperature is monitored to ensure the effectiveness and safety of the vehicle, and participates in 5 to 8% of the total drag and CO2 emissions. Dimensioning is an aerodynamic and aerothermal compromise, validated on a succession of road stages at constant speed and stopped phases (red lights, tolls, traffic jam). Although CFD is routinely used for forced convection, state-of-the-art turbulence models are not able to reproduce flows dominated by natural convection during stopped phases, with a Rayleigh number of the order of $10^{10}$, such that the design still relies on costly, full-scale, wind tunnel experiments. This technical barrier must be lifted, since the ambition of the PSA group is to reach a full digital design of their vehicles in the 2025 horizon, i.e., to almost entirely rely on CFD. This issue is the focus of the ongoing PhD thesis (CIFRE PSA) of S. Jameel, supervised by R. Manceau, and also a part of the ANR project MONACO_2025 described in section 9.2.2.

The Power & Vehicles Division of IFPEN co-develops the CFD code CONVERGE to simulate the internal flow in a spark-ignition engine, in order to provide the automotive industry with tools to optimize the design of combustion engines. The RANS method, widely used in the industry, is not sufficiently reliable for quantitative predictions, and is only used as a tool to qualitatively compare different geometries. On the other hand, LES provides more detailed and accurate information, but at the price of a CPU cost unaffordable for daily use in the industry. Therefore, IFPEN aims at developing the hybrid RANS/LES methodology, in order to combine the strengths of the two approaches. The just-started PhD thesis of Hassan Afailal, co-supervised by Rémi Manceau, is focused on this issue.

5. Highlights of the Year

5.1. ANR MONACO_2025

The MONACO_2025 proposal has been selected by ANR. In addition to Cagire, the consortium of this project, coordinated by [RM], consists in an academic partner, the institute PPrime of Poitiers, and two industrial partners, PSA and EDF. It is focused on the development of a CFD methodology for transient, buoyancy-affected turbulent flows, that are crucial for the two industrial partners. This project built up on the long-term collaboration with EDF, and the more recent collaboration with PSA through a master internship and the CIFRE PhD thesis of Saad Jameel.

5.2. First implementation of a turbulence model in AeroSol

In the long-term strategy of the CAGIRE team, the development of agile simulation, a first step towards auto-adaptive RANS/LES methods was made this summer during the internship of Axelle Perraud. This step consisted in the implementation in AeroSol of a first near-wall resolving turbulence model. Before focusing on innovative RANS and hybrid RANS/LES methods developed in CAGIRE, it was chosen to implement the standard, well-established $k-\omega$ RANS model, in order to make possible a straightforward validation in comparison with other CFD codes.
6. New Software and Platforms

6.1. AeroSol

**Keyword:** Finite element modelling

**Functional Description:** The AeroSol software is a high order finite element library written in C++. The code has been designed so as to allow for efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The work of the team CARDAMOM (previously Bacchus) is focused on continuous finite elements methods, while the team Cagire is focused on discontinuous Galerkin methods. However, everything is done for sharing the largest part of code we can. More precisely, classes concerning IO, finite elements, quadrature, geometry, time iteration, linear solver, models and interface with PaMPA are used by both of the teams. This modularity is achieved by mean of template abstraction for keeping good performances. The distribution of the unknowns is made with the software PaMPA, developed within the team TADAAM (and previously in Bacchus) and the team Castor.

**News of the Year:** The following points have been developed in the code

- A postprocessing in the high order GMSH format has been added
- On the Uhaina part, the work has been focused on the entropy viscosity approach for shock limiting, and on the positivity preserving limiters for ensuring positive water height
- On the dealing of low Mach problems - Multidimensional numerical flux accurate for the computation of steady and unsteady low Mach flows. - Test cases at low Mach
- A method for penalizing rigid bodies instead of meshing it has been developed within the postdoc of Marco Lorini. The model was implemented, an improvement of time schemes for steady problems was done. The method has been tested with 2d and 3d tests: bump, flow around a cylinder. These tests allowed to fix bugs, especially for wall boundary conditions. The coupling with adaptation tools has began.
- The library has benefited from the HPCLib Inria Hub, which aims at improving the development environment of HPC libraries within the Bordeaux Sud Ouest Centre. Within this project, a static analysis of the library based on sonarqube has been performed.
- A wiki for gathering the documentation of the different test cases has begun.
  - Participants: Benjamin Lux, Damien Genet, Dragan Amenga Mbengoue, Hamza Belkhayat Zougari, Mario Ricchiuto, Maxime Mogé, Simon Delmas and Vincent Perrier
  
**Contact:** Vincent Perrier

7. New Results

7.1. Development of an accurate and stable finite volume scheme for simulating low Mach number flows with or without acoustic waves

Starting from the Roe scheme and various low Mach fixes for the barotropic Euler PDE’s system and using a 2-scale asymptotic analysis of the (semi)-discrete system, a new Roe based scheme is derived whose set of dissipative terms is chosen in order to ensure both accuracy, stability and checkerboard free behaviour. A paper on this topic is being finalized.

7.2. Analysis of liquid sheet flowing under gravity

In the framework of an informal cooperation with Y. Le Guer and K. El Omari who are supervising the PhD thesis of A. Kacem, we have been involved in the experimental and the numerical study of liquid sheets falling under gravity [14]. The various flow regimes have been characterized in terms of the relevant dimensionless numbers (Weber, Reynolds, Ohnesorge) with a particular emphasis on the regimes leading to the appearance of holes within the liquid sheet. A journal paper has been submitted mid-2017 and is presently under revision.
7.3. First order hyperbolic formulation of dissipative systems

In the framework of the leave of Vincent Perrier at National institute of Aerospace, a general framework for defining first order formulation of nonlinear dissipative systems equipped with an entropy has been developed. The numerical methods for discretizing this type of system are still in development.

7.4. Improvement of turbulent heat flux modelling for buoyant flows

Several modifications were introduced in the Elliptic Blending Differential Flux Model (EB-DFM) to account for the influence of wall blockage on the turbulent heat flux. These modifications are introduced in order to reproduce, in association with the most recent version of the EB-RSM, the full range of regimes, from forced to natural convection, without any case-specific modification. The interest of the new model is demonstrated using analytical arguments, a priori tests and computations in channel flows in the different convection regimes, as well as in a differentially heated cavity. This work is published in *Int. J. Heat Fluid Flow* [10].

7.5. Modelling of turbulent flows with strong variations of the physical properties

The effects of a strong transverse temperature gradient, very common in industrial applications, on a turbulent Poiseuille flow were studied numerically using RANS models, in order to determine the closure level necessary to reproduce the influence of variations of the physical properties, for a wide range of wall-temperature ratios. Eddy-viscosity models prove able to correctly reproduce the asymmetry of the flow and the tendency toward relaminarization close to the hot wall, which are mainly due to the strong variations of the molecular viscosity. Discrepancies in the predictions of the different closure levels only appear for the highest temperature ratios. A journal paper is under revision for publication in *Int. J. Heat Fluid Flow*.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- EDF: "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", contract associated to the PhD thesis of Gaëtan Mangeon
- EDF: "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", contract associated to the PhD thesis of Vladimir Duffal
- IFPEN: "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", contract associated to the PhD thesis of Hassan Al AFAILAL

8.2. Bilateral Grants with Industry

- EDF (Cifre PhD grant): "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", PhD student: Gaëtan Mangeon
- EDF (Cifre PhD grant): "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", PhD student: Vladimir Duffal
- IFPEN (PhD grant): "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", PhD student: Hassan Al AFAILAL
- PSA (Cifre PhD grant): "Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", PhD student: Saad Jameel.
9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Predicting head losses in aeronautical fuel injectors

This is a 3-year programme, started mid-2015 and funded by Conseil Régional d’Aquitaine (2014 Call) and two small-size companies, AD Industrie (Gurmençon, France) and GDTECH (Bordes, France). The objective is to investigate the possibility of using advanced RANS or hybrid RANS-LES approaches to better predict the pressure losses in aeronautical fuel nozzles. [PB, RM]

9.1.2. SEIGLE

SEIGLE means “Simulation Expérimentation pour l’Interaction de Gouttes Liquides avec un Ecoulement fortement compressible”. It is a 3-year program which has started since October 2017 and was funded by Régional Nouvelle-Aquitaine, ISAE-ENSMA, CESTA and Inria. The interest of understanding aerodynamic mechanisms and liquid drops atomization is explained by the field of applications where they play a key role, specially in the new propulsion technologies through detonation in the aerospace as well as in the securities field. The SEIGLE project was articulated around a triptych experimentation, modeling and simulation. An experimental database will be constituted. It will rely on a newly installed facility (Pprime), similar to a supersonic gust wind tunnel/ hypersonic from a gaseous detonation tube at high pressure. This will allow to test modeling approaches (Pprime / CEA) and numerical simulation (Inria / CEA) with high order schemes for multiphase compressible flows, suitable for processing shock waves in two-phase media [VP, JJ].

9.2. National Initiatives

9.2.1. GIS Success

We are members of the CNRS GIS Success (Groupement d’Intérêt Scientifique) organised around two of the major CFD codes employed by the Safran group, namely AVBP and Yales 2. No scientific activity has been devoted around those codes during 2017 but Yales2 has been installed and tested on one of our workstation to prepare some planned scientific activity to come in 2018 in the field of low Mach flows and low Reynolds flows simulations [PB].

9.2.2. ANR MONACO_2025 [RM]

The ambition of the MONACO_2025 project, coordinated by Rémi Manceau, is to join the efforts made in two different industrial sectors in order to tackle the industrial simulation of transient, turbulent flows affected by buoyancy effects. It brings together two academic partners, the project-team Cagire hosted by the university of Pau, and the institute Pprime of the CNRS/ENSMA/university of Poitiers (PPRIME), and R&D departments of two industrial partners, the PSA group and the EDF group, who are major players of the automobile and energy production sectors, respectively.

- The main scientific objective of the project is to make a breakthrough in the unresolved issue of the modelling of turbulence/buoyancy interactions in transient situations, within the continuous hybrid RANS/LES paradigm, which consists in preserving a computational cost compatible with industrial needs by relying on statistical approaches where a fine-grained description of the turbulent dynamics is not necessary. The transient cavity flow experiments acquired during MONACO_2025 will provide the partners and the scientific community with an unrivalled source of knowledge of the physical mechanisms that must be accounted for in turbulence models.

- The main industrial objective is to make available computational methodologies to address dimensioning, reliability and security issues in buoyancy-affected transient flows. It is to be emphasized that such problems are not tackled using CFD at present in the industry. At the end of MONACO_2025, a panel of methodologies, ranging from simple URANS to sophisticated hybrid
model based on improved RANS models, will be evaluated in transient situations, against the dedicated cavity flow experiments and a real car underhood configuration. This final benchmark exercise will form a decision-making tool for the industrial partners, and will thus pave the way towards high-performance design of low-emission vehicles and highly secure power plants. In particular, the project is in line with the Full Digital 2025 ambition, e.g., the declared ambition of the PSA group to migrate, within the next decade, to a design cycle of new vehicles nearly entirely based on CAE (computer aided engineering), without recourse to expensive full-scale experiments.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. SOPRANO

Participants: Rémi Manceau, Pascal Bruel, [Post doc starting in 2018].

Topic: MG-1.2-2015 - Enhancing resource efficiency of aviation

Project acronym: SOPRANO

Project title: Soot Processes and Radiation in Aeronautical inNOvative combustors

Duration: 01/09/2016 - 31/08/2020

Coordinator: SAFRAN

Other partners:
- France: CNRS, CERFACS, INSA Rouen, SAFRAN SA, Snecma SAS, Turbomeca SA.
- Germany: DLR, GE-DE Gmbh, KIT, MTU, RRD,
- Italy: GE AVIO SRL, University of Florence
- United Kingdom: Rolls Royce PLC, Imperial College of Science, Technology and Medecine, Loughborough University.

Abstract: For decades, most of the aviation research activities have been focused on the reduction of noise and NOx and CO2 emissions. However, emissions from aircraft gas turbine engines of non-volatile PM, consisting primarily of soot particles, are of international concern today. Despite the lack of knowledge toward soot formation processes and characterization in terms of mass and size, engine manufacturers have now to deal with both gas and particles emissions. Furthermore, heat transfer understanding, that is also influenced by soot radiation, is an important matter for the improvement of the combustor’s durability, as the key point when dealing with low-emissions combustor architectures is to adjust the air flow split between the injection system and the combustor’s walls. The SOPRANO initiative consequently aims at providing new elements of knowledge, analysis and improved design tools, opening the way to: • Alternative designs of combustion systems for future aircrafts that will enter into service after 2025 capable of simultaneously reducing gaseous pollutants and particles, • Improved liner lifetime assessment methods. Therefore, the SOPRANO project will deliver more accurate experimental and numerical methodologies for predicting the soot emissions in academic or semi-technical combustion systems. This will contribute to enhance the comprehension of soot particles formation and their impact on heat transfer through radiation. In parallel, the durability of cooling liner materials, related to the walls air flow rate, will be addressed by heat transfer measurements and predictions. Finally, the expected contribution of SOPRANO is to apply these developments in order to determine the main promising concepts, in the framework of current low-NOx technologies, able to control the emitted soot particles in terms of mass and size over a large range of operating conditions without compromising combustor’s liner durability and performance toward NOx emissions.

In the SOPRANO project, our objective is to complement the experimental (ONERA) and LES (CERFACS) work by RANS computations of the flow around a multiperforated plate, in order to build a database making possible a parametric study of mass, momentum and heat transfer through the plate and the development of multi-parameter-dependent equivalent boundary conditions. Our activity is due to start in September 2018.
9.4. International Initiatives

9.4.1. Informal International Partners

- Collaboration with Alireza Mazaheri, from NASA Langley Research Center on the first order formulation of the compressible Navier-Stokes system (2-month leave of V. Perrier at National Institute of Aerospace, Hampton, VA).
- Collaboration with E. Dick (University of Ghent, Belgium) and Y. Moguen (UPPA) on the determination of the best splitting of variables for handling low Mach flows with a pressure-energy based coupling. [PB]
- Collaboration with A. Beketaeva and A. Naïmanova (Institute of Mathematics, Almaty, Kazakhstan) related to the simulations of a supersonic jet in crossflow configuration. Contacts were also made with Axel Vincent from Onera Palaiseau in order to have access to recent experimental data on supersonic combustion. The low-Mach preconditioning of an in-house ENO based compressible flow solver was also addressed. [PB] (10-day stay in Almaty).
- Collaboration with P. Correia (University of Evora, Portugal) related to the development of enhanced boundary conditions for the simulations of Mach zero flows with the artificial compressibility method. [PB] (5-day stay in Evora).
- Collaboration with S. Lardeau (Siemens Industry Software Computational Dynamics, Nuremberg, Germany) on the EB-RSM model and hybrid RANS/LES model for industrial applications. [RM]

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Prof. Sergio Elaskar (Conicet and University National of Cordoba, Argentina) visited LMAP-Cagire for a 1-week stay from August 28 to September 1, 2017.
- Prof. Ezequiel Del Rio (Polytechnic University of Madrid) visited LMAP-Cagire for a 4-day stay from August 21 to August 31, 2017. The objective of these two simultaneous visits was to determine the possibility of generating data on the Maveric test facility to validate the intermittency model (mapping) jointly developed by S. Elaskar and E. Del Rio.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- Member [RM] of the steering committee of the Special Interest Group “Turbulence Modelling” (SIG-15) of ERCOFTAC (European Research COmmittee for Flow, Turbulence and Combustion) that organizes a series of international workshops dedicated to cross-comparisons of the results of turbulence models and experimental/DNS databases.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

- ASME 2018 Fluids Engineering Division Summer Meeting (FEDSM) [RM]

10.1.2.2. Reviewer

This year, the team members have reviewed (3) contributions for the following conferences:

- ASME-GT Turbo Expo 2018 (Oslo, Norway) (1) [PB]
- FVCA 2017 (Lille, France) (1) [JJ]
- REEEE 2017 (Fez, Marocco) (1) [PB]
10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Visualization of Mechanical Processes [PB]
- Advisory Board of International Journal of Heat and Fluid Flow [RM]
- Advisory Board of Flow, Turbulence and Combustion [RM]

10.1.3.2. Reviewer - Reviewing Activities

During 2017, the team members reviewed (13) papers for the following journals:

- Combustion and Flame (3) [PB]
- Compte Rendus Mécanique (1) [PB]
- Energy and Buildings (1) [PB]
- International Journal of Fluid Mechanics Research (1) [PB]
- International Journal of Heat and Fluid Flow (2) [RM]
- Journal of Petroleum Science and Engineering (1) [PB]
- Mathematics and Computers in Simulation (1) [RM]
- Nuclear Eng Design (2) [RM]
- Physics of fluids (1) [RM]

10.1.4. Research Administration

- Co-responsible of seventh day of welcoming new recruits at Institut Henri Poincaré on January [JJ]
- Co-responsible of the organisation of the LMAP seminar [JJ]
- Member of the LMAP council [PB]
- Member of the IPRA scientific council [RM]

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master : "Maths 2: Data analysis", 68h25, M1 - Génie Pétrolier, Université de Pau et des Pays de l’Adour, Pau, France. [JJ]
Master : "Finite volume for hyperbolic systems and compressible fluid mechanics", 26h25, M2 - MMS, Université de Pau et des Pays de l’Adour, Pau, France. [JJ]
Master : "Finite volume for hyperbolic systems and compressible fluid mechanics", 24h75, M2 - MMS, Université de Pau et des Pays de l’Adour, Pau, France. [VP]
Master : “Turbulence modelling” (in English), 27h30, M2 - International Master program Turbulence, Université de Poitiers/Ecole centrale de Lille, France. [RM]
Eng. 3 : “Industrial codes for CFD” (in English), 12h30, 3rd year of engineering school (M2), ENSMA, Poitiers, France. [RM]
Eng. 3 : “Advanced physics–Turbulence modelling for CFD”, 16h, 3rd year of engineering school (M2), ENSGTI, France. [RM]

10.2.2. Supervision

PhD in progress: Gaetan Mangeon, "Modelisation avancée des transferts thermiques pour les configurations industrielles avec et sans prise en compte de la paroi solide", 2017 Supervisor: [RM].
PhD in progress: Saad Jamel, "Modélisation de la turbulence en régimes de convection mixte et naturelle dans un contexte automobile", 2017, Supervisor: [RM].

0http://lma-umr5142.univ-pau.fr/fr/activites-scientifiques/seminaires/seminaires-math-et-applications.html
10.2.3. Juries

The participation in the following thesis juries is noted ("referee" in a French doctoral thesis jury is more or less equivalent to an external opponent in an Anglo-Saxon like PhD jury):

PhD: Océane Lambert «Solutions architecturées par fabrication additive pour le refroidissement de parois de chambres de combustion» Communauté Université Grenoble Alpes, France, 17 October 2017. Supervisors: R. Dendeviel - C. Davoine. [PB, referee]

10.3. Popularization

- "Forum des Métiers" organized by "Collège Pierre Emmanuel", Pau (64), France, 18 May 2017. A stand was manned during one day with the objective of explaining the activity of researcher to an audience of middle school students. [PB]

11. Bibliography

Major publications by the team in recent years


Publications of the year

Articles in International Peer-Reviewed Journal


Invited Conferences


International Conferences with Proceedings


Conferences without Proceedings


Other Publications


[16] P. BRUEL. The simulation of low Mach flows: from the AUSM-IT flux scheme to ATCBC boundary conditions, March 2017, Seminar - Universidad Nacional de Córdoba - Argentina, https://hal.inria.fr/hal-01651971.

[17] V. PERRIER. A task-driven implementation of a simple numerical solver for hyperbolic conservation laws, February 2017, NASA LaRC HPC Seminar, https://hal.inria.fr/hal-01668927.
References in notes


Project-Team CARDAMOM

Certified Adaptive discRete moDels for robust simulAtions of CoMplex flOws with Moving fronts

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations
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Project-Team CARDAMOM

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 June 01

Keywords:

Computer Science and Digital Science:
- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.4. - Multiscale modeling
- A6.1.5. - Multiphysics modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.2.6. - Optimization
- A6.2.8. - Computational geometry and meshes
- A6.3.1. - Inverse problems
- A6.3.4. - Model reduction
- A6.3.5. - Uncertainty Quantification

Other Research Topics and Application Domains:
- B3.3.2. - Water: sea & ocean, lake & river
- B3.3.3. - Littoral
- B3.4.1. - Natural risks
- B4.3.2. - Hydro-energy
- B5.2.1. - Road vehicles
- B5.2.3. - Aviation
- B5.2.4. - Aerospace
- B5.5. - Materials

1. Personnel

Research Scientists
- Mario Ricchiuto [Team leader, Inria, Senior Researcher]
- Pietro Marco Congedo [Inria, Researcher, HDR]
- Maria Kazolea [Inria, Researcher]

Faculty Members
- Heloise Beaugendre [Institut National Polytechnique de Bordeaux, Associate Professor, HDR]
- Mathieu Colin [Institut National Polytechnique de Bordeaux, Associate Professor, HDR]
- Cecile Dobrzynski [Institut National Polytechnique de Bordeaux, Associate Professor]
- Fabien Marche [Univ de Montpellier, Associate Professor, from Sep 2017, HDR]
- Luc Mieussens [Institut National Polytechnique de Bordeaux, Professor]

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2. Overall Objectives

2.1. Overall Objectives

CARADAMOM is a joint team of Inria Bordeaux - Sud-Ouest, University of Bordeaux and Bordeaux Inst. Nat. Polytechnique) and IMB (Institut de Mathématiques de Bordeaux – CNRS UMR 5251, University of Bordeaux). CARADAMOM has been created on January 1\textsuperscript{st}, 2015 (https://team.inria.fr/crardamom/). The CARADAMOM project aims at providing a robust modelling strategy for engineering applications involving complex flows with moving fronts. The term front here denotes either an actual material boundary (e.g. multiple phases), a physical discontinuity (e.g. shock waves), or a transition layer between regions with completely different dominant flow behaviour (e.g. breaking waves). These fronts introduce a multi-scale behaviour. The resolution of all the scales is however not feasible in certification and optimization cycles, and not necessary in many engineering applications, while in others it is enough to model the average effect of small scales on large ones (closure models). We plan to develop application-tailored models obtained by a tight combination of asymptotic PDE (Partial Differential Equations) modelling, adaptive high order PDE discretizations, and a quantitative certification step assessing the sensitivity of outputs to both model components (equations, numerical methods, etc) and random variations of the data. The goal is to improve parametric analysis and design cycles, by increasing both accuracy and confidence in the results thanks to improved physical and numerical modelling, and to a quantitative assessment of output uncertainties. This requires a research program mixing of PDE analysis, high order discretizations, Uncertainty Quantification (UQ), robust optimization, and some specific engineering know how. Part of these scientific activities started in the BACCHUS and MC2 teams. CARADAMOM harmonizes and gives new directions to this know how.

2.2. Scientific context and challenges

The objective of this project is to provide improved analysis and design tools for engineering applications involving fluid flows, and in particular flows with moving fronts. In our applications a front is either an actual material interface, or a well identified and delimited transition region in which the flow undergoes a change in its dominant macroscopic character. One example is the certification of wing de anti-icing systems, involving the predictions of ice formation and detachment, and of ice debris trajectories to evaluate the risk of downstream impact on aircraft components [138], [64]. Another application, relevant for space reentry, is the study of transitional regimes in high altitude gas dynamics in which extremely thin layers appear in the flow which cannot be analysed with classical continuous models (Navier-Stokes equations) used by engineers [72], [99]. An important example in coastal engineering is the transition between propagating and breaking waves, characterized by a strong local production of vorticity and by dissipative effects absent when waves propagates [74]. Similar examples in energy and material engineering provide the motivation of this project.
All these application fields involve either the study of new technologies (e.g. new design/certification tools for aeronautics [80], [94], [113], [64] or for wave energy conversion [91]), or parametric studies of complex environments (e.g. harbour dynamics [102], or estuarine hydrodynamics [59]), or hazard assessment and prevention [96]. In all cases, computationally affordable, quick, and accurate numerical modelling is essential to improve the quality of (or to shorten) design cycles and allow performance level enhancements in early stages of development [143]. The goal is to afford simulations over very long times with many parameters or to embed a model in an alert system.

In addition to this, even in the best of circumstances, the reliability of numerical predictions is limited by the intrinsic randomness of the data used in practice to define boundary conditions, initial conditions, geometry, etc. This uncertainty, related to the measurement errors, is defined as aleatory, and cannot be removed, nor reduced. In addition, physical models and the related Partial Differential Equations (PDEs), feature a structural uncertainty, since they are derived with assumptions of limited validity and calibrated with manipulated experimental data (filtering, averaging, etc.). These uncertainties are defined as epistemic, as they are a deficiency due to a lack of knowledge [54], [126]. Unfortunately, measurements in fluids are delicate and expensive. In complex flows, especially in flows involving interfaces and moving fronts, they are sometimes impossible to carry out, due to scaling problems, repeatability issues (e.g. tsunami events), technical issues (different physics in the different flow regions) or dangerousness (e.g. high temperature reentry flows, or combustion). Frequently, they are impractical, due to the time scales involved (e.g. characterisation of oxidation processes related to a new material micro-/meso- structure [82]). This increases the amount of uncertainties associated to measurements and reduces the amount of information available to construct physical/PDE models. These uncertainties play also a crucial role when one wants to deal with numerical certification or optimization of a fluid based device. However, this makes the required number of flow simulations grow as high as hundreds or even thousands of times. The associated costs are usually prohibitive. So the real challenge is to be able to construct an accurate and computationally affordable numerical model handling efficiently uncertainties. In particular, this model should be able to take into account the variability due to uncertainties, those coming from the certification/optimization parameters as well as those coming from modelling choices.

To face this challenge and provide new tools to accurately and robustly modelize and certify engineering devices based on fluid flows with moving fronts, we propose a program mixing scientific research in asymptotic PDE analysis, high order adaptive PDE discretizations and uncertainty quantification.

2.3. Our approach

A standard way a certification study may be contacted can be described as two box modelling. The first box is the physical model itself, which is composed of the 3 main elements: PDE system, mesh generation/adaptation, and discretization of the PDE (numerical scheme). The second box is the main robust certification loop which contains separate boxes involving the evaluation of the physical model, the post-processing of the output, and the exploration of the spaces of physical and stochastic parameters (uncertainties). There are some known interactions taking place in the loop which are a necessary to exploit as much as possible the potential of high order methods [105] such as e.g. $h-/p-/r-$ adaptation in the physical model w.r.t. some post-processed output value, or w.r.t. some sort of adjoint sensitivity coming from the physical parameter evolution box, etc. As things stand today, we will not be able to take advantage of the potential of new high order numerical techniques and of hierarchical (multi-fidelity) robust certification approaches without some very aggressive adaptive methodology. Such a methodology, will require interactions between e.g. the uncertainty quantification methods and the adaptive spatial discretization, as well as with the PDE modelling part. Such a strategy cannot be developed, let alone implemented in an operational context, without completely disassembling the scheme of the two boxes, and letting all the parts (PDE system, mesh generation/adaptation, numerical scheme, evaluation of the physical model, the post processing of the output, exploration of the spaces of physical and stochastic parameters) interact together. This is what we want to do in CARDAMOM. We have the unique combination of skills which allows to explore such an avenue: PDE analysis, high order numerical discretizations, mesh generation and adaptation, optimization and uncertainty quantification, specific issues related to the applications considered.
Our strength is also our unique chance of exploring the interactions between all the parts. We will try to answer some fundamental questions related to the following aspects:

- What are the relations between PDE model accuracy (asymptotic error) and scheme accuracy, and how to control, or possibly exploit these relations to minimize the error for a given computational effort;
- How to devise and implement adaptation techniques ($r-$, $h-$, and $p-$) for time dependent problems while guaranteeing an efficient time marching procedure (minimize CPU time at constant error);
- How to exploit the wide amount of information made available from the optimization and uncertainty quantification process to construct a more aggressive adaptation strategy in physical, parameter, and stochastic space, and in the physical model itself.

These research avenues related to the PDE models and numerical methods used, will allow us to have an impact on the applications communities targeted which are:

- Aeronautics and aerospace engineering (de-anti icing systems, space re-entry);
- Energy engineering (organic Rankine cycles and wave energy conversion);
- Material engineering (self healing composite materials);
- Coastal engineering (coastal protection, hazard assessment etc.).

The main research directions related to the above topics are discussed in the following section.

## 3. Research Program

### 3.1. Variational discrete asymptotic modelling

In many of the applications we consider, intermediate fidelity models are or can be derived using an asymptotic expansion for the relevant scale resolving PDEs, and eventually considering some averaged for of the resulting continuous equations. The resulting systems of PDEs are often very complex and their characterization, e.g. in terms of stability, unclear, or poor, or too complex to allow to obtain discrete analogy of the continuous properties. This makes the numerical approximation of these PDE systems a real challenge. Moreover, most of these models are often based on asymptotic expansions involving small geometrical scales. This is true for many applications considered here involving flows in/of thin layers (free surface waves, liquid films on wings generating ice layers, oxide flows in material cracks, etc). This asymptotic expansion is nothing else than a discretization (some sort of Taylor expansion) in terms of the small parameter. The actual discretization of the PDE system is another expansion in space involving as a small parameter the mesh size. What is the interaction between these two expansions? Could we use the spatial discretization (truncation error) as means of filtering undesired small scales instead of having to explicitly derive PDEs for the large scales? We will investigate in depth the relations between asymptotics and discretization by:

- comparing the asymptotic limits of discretized forms of the relevant scale resolving equations with the discretization of the analogous continuous asymptotic PDEs. Can we discretize a well understood system of PDEs instead of a less understood and more complex one?
- study the asymptotic behaviour of error terms generated by coarse one-dimensional discretization in the direction of the “small scale”. What is the influence of the number of cells along the vertical direction, and of their clustering?
- derive equivalent continuous equations (modified equations) for anisotropic discretizations in which the direction is direction of the “small scale” is approximated with a small number of cells. What is the relation with known asymptotic PDE systems?
Our objective is to gain sufficient control of the interaction between discretization and asymptotics to be able to replace the coupling of several complex PDE systems by adaptive strongly anisotropic finite element approximations of relevant and well understood PDEs. Here the anisotropy is intended in the sense of having a specific direction in which a much poorer (and possibly variable with the flow conditions) polynomial approximation (expansion) is used. The final goal is, profiting from the availability of faster and cheaper computational platforms, to be able to automatically control numerical and physical accuracy of the model with the same techniques. This activity will be used to improve our modelling in coastal engineering as well as for de-anti icing systems, wave energy converters, composite materials (cf. next sections).

In parallel to these developments, we will make an effort in to gain a better understanding of continuous asymptotic PDE models. We will in particular work on improving, and possibly, simplifying their numerical approximation. An effort will be done in trying to embed in these more complex nonlinear PDE models discrete analogs of operator identities necessary for stability (see e.g. the recent work of [108], [112] and references therein).

3.2. High order discretizations on moving adaptive meshes

We will work on both the improvement of high order mesh generation and adaptation techniques, and the construction of more efficient, adaptive high order discretisation methods.

Concerning curved mesh generation, we will focus on two points. First propose a robust and automatic method to generate curved simplicial meshes for realistic geometries. The untangling algorithm we plan to develop is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. Second we plan to extend the method proposed in [57] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the initial results of [61], [63] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [122], [134], [75]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [57], and with improved algorithms to discretize accurately and fast the elliptic equations involved. For this we will explore different type of relaxation methods, including those proposed in [110], [115], [114] allowing to re-use high order discretizations techniques already used for the flow variables. All these modelling approaches for the mesh movement are based on some minimization argument, and do not allow easily to take into account explicitly properties such as e.g. the positivity of nodal volumes. An effort will be made to try to embed these properties, as well as to improve the control on the local mesh sizes obtained. Developments made in numerical methods for Lagrangian hydrodynamics and compressible materials may be a possible path for these objectives (see e.g. [87], [141], [139] and references therein). We will stretch the use of these techniques as much as we can, and couple them with remeshing algorithms based on local modifications plus conservative, high order, and monotone ALE (or other) remaps (cf. [58], [97], [142], [84] and references therein).

The development of high order schemes for the discretization of the PDE will be a major part of our activity. We will work from the start in an Arbitrary Lagrangian Eulerian setting, so that mesh movement will be easily accommodated, and investigate the following main points:

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [63], [61]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;
the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, an the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels\cite{62}. Similar problems may arise in other applications. Possible solutions to this competition may come from super-approximation (use of higher order polynomials) of some of the data allowing to reduce (e.g. bathymetry) the error in the preservation of one of the competing quantities. This is similar to what is done in super-parametric approximations of the boundaries of an object immersed in the flow, except that in our case the data may enter the PDE explicitly and not only through the boundary conditions. Several efficient solutions for this issue will be investigated to obtain fully conservative moving mesh approaches:

- an issue related to the previous one is the accurate treatment of wall boundaries. It is known that even for standard lower order (second) methods, a higher order, curved, approximation of the boundaries may be beneficial. This, however, may become difficult when considering moving objects, as in the case e.g. of the study of the impact of ice debris in the flow. To alleviate this issue, we plan to follow on with our initial work on the combined use of immersed boundaries techniques with high order, anisotropic (curved) mesh adaptation. In particular, we will develop combined approaches involving high order hybrid meshes on fixed boundaries with the use of penalization techniques and immersed boundaries for moving objects. We plan to study the accuracy obtainable across discontinuous functions with $r$-adaptive techniques, and otherwise use whenever necessary anisotropic meshes to be able to provide a simplified high order description of the wall boundary (cf.\cite{107}). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body\cite{113,116}. An effort will be also made on improving the accuracy of these techniques using e.g. higher order approaches, either based on generalizations of classical splitting methods\cite{98}, or on some iterative Defect Correction method (see e.g.\cite{77});

- the proper treatment of different physics may be addressed by using mixed/hybrid schemes in which different variables/equations are approximated using a different polynomial expansion. A typical example is our work on the discretization of highly non-linear wave models\cite{93} in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such methods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms;

- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results\cite{124,60,125} to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni\cite{76}, allowing to have a more flexible approach similar to the so-called $P^rP^m$ method\cite{90,130}. How to localize these enhancements, and to efficiently perform local reconstructions/enrichment, as well as $p$--adaptation, and handling hanging nodes will also be a main line of work. A clever combination of hierarchical enrichment of the polynomials, with a constrained approximation will be investigated. All these developments will be combined with the shock capturing/positivity preserving construction we
developed in the past. Other discontinuity resolving techniques will be investigated as well, such as face limiting techniques as those partially studied in [95];

- time stepping is an important issue, especially in presence of local mesh adaptation. The techniques we use will force us to investigate local and multilevel techniques. We will study the possibility constructing semi-implicit methods combining extrapolation techniques with space-time variational approaches. Other techniques will be considered, as multi-stage type methods obtained using Defect-Correction, Multi-step Runge-Kutta methods [73], as well as spatial partitioning techniques [104]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

As already remarked, classical methods for uncertainty quantification are affected by the so-called Curse-of-Dimensionality. Adaptive approaches proposed so far, are limited in terms of efficiency, or of accuracy. Our aim here is to develop methods and algorithms permitting a very high-fidelity simulation in the physical and in the stochastic space at the same time. We will focus on both non-intrusive and intrusive approaches.

Simple non-intrusive techniques to reduce the overall cost of simulations under uncertainty will be based on adaptive quadrature in stochastic space with mesh adaptation in physical space using error monitors related to the variance of to the sensitivities obtained e.g. by an ANOVA decomposition. For steady state problems, remeshing using metric techniques is enough. For time dependent problems both mesh deformation and remeshing techniques will be used. This approach may be easily used in multiple space dimensions to minimize the overall cost of model evaluations by using high order moments of the properly chosen output functional for the adaptation (as in optimization). Also, for high order curved meshes, the use of high order moments and sensitivities issued from the UQ method or optimization provides a viable solution to the lack of error estimators for high order schemes.

Despite the coupling between stochastic and physical space, this approach can be made massively parallel by means of extrapolation/interpolation techniques for the high order moments, in time and on a reference mesh, guaranteeing the complete independence of deterministic simulations. This approach has the additional advantage of being feasible for several different application codes due to its non-intrusive character.

To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten’s multiresolution framework, following [56]. This framework allows a reduction of the dimensionality of the discrete space of function representation, defined in a proper stochastic space. This reduction allows a reduction of the number of explicit evaluations required to represent the function, and thus a gain in efficiency. Moreover, multiresolution analysis offers a natural tool to investigate the local regularity of a function and can be employed to build an efficient refinement strategy, and also provides a procedure to refine/coarsen the stochastic space for unsteady problems. This strategy should allow to capture and follow all types of flow structures, and, as proposed in [56], allows to formulate a non-linear scheme in terms of compression capabilities, which should allow to handle non-smooth problems. The potential of the method also relies on its moderate intrusive behaviour, compared to e.g. spectral Galerkin projection, where a theoretical manipulation of the original system is needed.

Several activities are planned to generalize our initial work, and to apply it to complex flows in multiple (space) dimensions and with many uncertain parameters.

The first is the improvement of the efficiency. This may be achieved by means of anisotropic mesh refinement, and by experimenting with a strong parallelization of the method. Concerning the first point, we will investigate several anisotropic refinement criteria existing in literature (also in the UQ framework), starting with those already used in the team to adapt the physical grid. Concerning the implementation, the scheme formulated in [56] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the
scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

Another main objective is related to the use of multiresolution in both physical and stochastic space. This requires a careful handling of data and an updated definition of the wavelet. Until now, only a weak coupling has been performed, since the number of points in the stochastic space varies according to the physical space, but the number of points in the physical space remains unchanged. Several works exist on the multiresolution approach for image compression, but this could be the first time in which this kind of approach would be applied at the same time in the two spaces with an unsteady procedure for refinement (and coarsening). The experimental code developed using these technologies will have to fully exploit the processing capabilities of modern massively parallel architectures, since there is a unique mesh to handle in the coupled physical/stochastic space.

3.4. Robust multi-fidelity modelling for optimization and certification

Due to the computational cost, it is of prominent importance to consider multi-fidelity approaches gathering high-fidelity and low-fidelity computations. Note that low-fidelity solutions can be given by both the use of surrogate models in the stochastic space, and/or eventually some simplified choices of physical models of some element of the system. Procedures which deal with optimization considering uncertainties for complex problems may require the evaluation of costly objective and constraint functions hundreds or even thousands of times. The associated costs are usually prohibitive. For these reason, the robustness of the optimal solution should be assessed, thus requiring the formulation of efficient methods for coupling optimization and stochastic spaces. Different approaches will be explored. Work will be developed along three axes:

1. a robust strategy using the statistics evaluation will be applied separately, i.e. using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex\(^2\) method \[81\];
2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model;
3. develop advanced methods for robust optimization. In particular, the Simplex\(^2\) method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

This work is related to the activities foreseen in the EU contract MIDWEST, in the ANR LabCom project VIPER (currently under evaluation), in a joint project with DGA and VKI, in two projects under way with AIRBUS and SAFRAN-HERAKLES.

4. Application Domains

4.1. De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice
pieces do not significantly affect the flow. The second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immerse boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [65] it has been proposed to model ice shedding trajectories by an innovative paradigm that is based on CArtesian grids, PEnalization and LEvel Sets (LESCAPE code). Our objective is to use the potential of high order unstructured mesh adaptation and immersed boundary techniques to provide a geometrically flexible extension of this idea. These activities will be linked to the development of efficient mesh adaptation and time stepping techniques for time dependent flows, and their coupling with the immersed boundary methods we started developing in the FP7 EU project STORM [55], [116]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [88], [106], [107]. From the numerical point of view one of the major challenges is to guarantee efficiency and accuracy of the time stepping in presence of highly stretched adaptive and moving meshes. Semi-implicit, locally implicit, multi-level, and split discretizations will be explored to this end.

Besides the numerical aspects, we will deal with modelling challenges. One source of complexity is the initial conditions which are essential to compute ice shedding trajectories. It is thus extremely important to understand the mechanisms of ice release. With the development of next generations of engines and aircraft, there is a crucial need to better assess and predict icing aspects early in design phases and identify breakthrough technologies for ice protection systems compatible with future architectures. When a thermal ice protection system is activated, it melts a part of the ice in contact with the surface, creating a liquid water film and therefore lowering ability of the ice block to adhere to the surface. The aerodynamic forces are then able to detach the ice block from the surface [67]. In order to assess the performance of such a system, it is essential to understand the mechanisms by which the aerodynamic forces manage to detach the ice. The current state of the art in icing codes is an empirical criterion. However such an empirical criterion is unsatisfactory. Following the early work of [71], [64] we will develop appropriate asymptotic PDE approximations allowing to describe the ice formation and detachment, trying to embed in this description elements from damage/fracture mechanics. These models will constitute closures for aerodynamics/RANS and URANS simulations in the form of PDE wall models, or modified boundary conditions.

In addition to this, several sources of uncertainties are associated to the ice geometry, size, orientation and the shedding location. In very few papers [120], some sensitivity analysis based on Monte Carlo method have been conducted to take into account the uncertainties of the initial conditions and the chaotic nature of the ice particle motion. We aim to propose some systematic approach to handle every source of uncertainty in an efficient way relying on some state-of-art techniques developed in the Team. In particular, we will perform an uncertainty propagation of some uncertainties on the initial conditions (position, orientation, velocity,...) through a low-fidelity model in order to get statistics of a multitude of particle tracks. This study will be done in collaboration with ETS (Ecole de Technologies Supérieure, Canada). The longterm objective is to produce footprint maps and to analyse the sensitivity of the models developed.

4.2. Space re-entry

As already mentioned, atmospheric re-entry involves multi-scale fluid flow physics including highly rarefied effects, aerothermochemistry, radiation. All this must be coupled to the response of thermal protection materials to extreme conditions. This response is most often the actual objective of the study, to allow the certification of Thermal Protection Systems (TPS).
One of the applications we will consider is the so-called post-flight analysis of a space mission. This involves
reconstructing the history of the re-entry module (trajectory and flow) from data measured on the spacecraft
by means of a Flush Air Data System (FADS), a set of sensors flush mounted in the thermal protection
system to measure the static pressure (pressure taps) and heat flux (calorimeters). This study involves the
accurate determination of the freestream conditions during the trajectory. In practice this means determining
temperature, pressure, and Mach number in front of the bow shock forming during re-entry. As shown by
zur Nieden and Olivier [145], state of the art techniques for freestream characterization rely on several
approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account
the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement
errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas
surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects
and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation,
on the chemical model parameters in the bulk and at the wall (surface catalysis).

Rebuilding the freestream conditions from the stagnation point data therefore amounts to solving a stochastic
inverse problem, as in robust optimization. Our objective is to build a robust and global framework for
rebuilding freestream conditions from stagnation-point measurements for the trajectory of a re-entry vehicle.
To achieve this goal, methods should be developed for

- an accurate simulation of the flow in all the regimes, from rarefied, to transitional, to continuous ;
- providing a complete analysis about the reliability and the prediction of the numerical simulation
  in hypersonic flows, determining the most important source of error in the simulation (PDE model, 
  discretization, mesh, etc)
- reducing the overall computational cost of the analysis .

Our work on the improvement of the simulation capabilities for re-entry flows will focus both on the models
and on the methods. We will in particular provide an approach to extend the use of standard CFD models in
the transitional regime, with CPU gains of several orders of magnitude w.r.t. Boltzmann solvers. To do this
we will use the results of a boundary layer analysis allowing to correct the Navier-Stokes equations. This
theory gives modified (or extended) boundary conditions that are called "slip velocity" and "temperature
jump" conditions. This theory seems to be completely ignored by the aerospace engineering community.
Instead, people rather use a simpler theory due to Maxwell that also gives slip and jump boundary conditions:
however, the coefficients given by this theory are not correct. This is why several teams have tried to modify
these coefficients by some empirical methods, but it seems that this does not give any satisfactory boundary
conditions.

Our project is twofold. First, we want to revisit the asymptotic theory, and to make it known in the aerospace
community. Second, we want to make an intensive sensitivity analysis of the model to the various coefficients
of the boundary conditions. Indeed, there are two kinds of coefficients in these boundary conditions. The
first one is the accommodation coefficient: in the kinetic model, it gives the proportion of molecules that are
 specularly reflected, while the others are reflected according to a normal distribution (the so-called diffuse
reflection). This coefficient is a data of the kinetic model that can be measured by experiments: it depends on
the material and the structure of the solid boundary, and of the gas. Its influence on the results of a Navier-
Stokes simulation is certainly quite important. The other coefficients are those of the slip and jump boundary
conditions: they are issued from the boundary layer analysis, and we have absolutely no idea of the order of
magnitude of their influence on the results of a Navier-Stokes solution. In particular, it is not clear if these
results are more sensitive to the accommodation coefficient or to these slip and jump coefficients.

In this project, we shall make use of the expertise of the team on uncertainty quantification to investigate
the sensitivity of the Navier-Stokes model with slip and jump coefficients to these various coefficients. This
would be rather new in the field of aerospace community. It could also have some impacts in other sciences
in which slip and jump boundary conditions with incorrect coefficients are still used, like for instance in spray
simulations: for very small particles immersed in a gas, the drag coefficient is modified to account for rarefied
effects (when the radius of the particle is of the same order of magnitude as the mean free path in the gas), and
slip and jump boundary conditions are used.
Another application which has very close similarities to the physics of de-anti icing systems is the modelling of the solid and liquid ablation of the thermal protective system of the aircraft. This involves the degradation and recession of the solid boundary of the protection layer due to the heating generated by the friction. As in the case of de-anti icing systems, the simulation of these phenomena need to take into account the heat conduction in the solid, its phase change, and the coupling between a weakly compressible and a compressible phase. Fluid/Solid coupling methods are generally based on a weak approach. Here we will both study, by theoretical and numerical techniques, a strong coupling method for the interaction between the fluid and the solid, and, as for de-anti icing systems, attempt at developing appropriate asymptotic models. These would constitute some sort of thin layer/wall models to couple to the external flow solver.

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [68], [111]. These tools will be coupled to our robust inverse techniques. One of our objectives is to development of a low-cost strategy for improving the numerical prediction by taking into account experimental data. Some methods have been recently introduced [119] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework sing the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

These activities will benefit from our strong collaborations with the CEA and with the von Karman Institute for Fluid Dynamics and ESA.

4.3. Energy

We will develop modelling and design tools, as well as dedicated platforms, for Rankine cycles using complex fluids (organic compounds), and for wave energy extraction systems. Organic Rankine Cycles (ORCs) use heavy organic compounds as working fluids. This results in superior efficiency over steam Rankine cycles for source temperatures below 900 K. ORCs typically require only a single-stage rotating component making them much simpler than typical multi-stage steam turbines. The strong pressure reduction in the turbine may lead to supersonic flows in the rotor, and thus to the appearance of shocks, which reduces the efficiency due to the associated losses. To avoid this, either a larger multi stage installation is used, in which smaller pressure drops are obtained in each stage, or centripetal turbines are used, at very high rotation speeds (of the order of 25,000 rpm). The second solution allows to keep the simplicity of the expander, but leads to poor turbine efficiencies (60-80%) w.r.t. modern, highly optimized, steam and gas turbines - and to higher mechanical constraints. The use of dense-gas working fluids, i.e. operating close to the saturation curve, in properly chosen conditions could increase the turbine critical Mach number avoiding the formation of shocks, and increasing the efficiency. Specific shape optimization may enhance these effects, possibly allowing the reduction of rotation speeds. However, dense gases may have significantly different properties with respect to dilute ones. Their dynamics is governed by a thermodynamic parameter known as the fundamental derivative of gas dynamics

$$\Gamma = 1 + \frac{\rho}{c} \left( \frac{\partial c}{\partial \rho} \right)_s,$$

where $\rho$ is the density, $c$ is the speed of sound and $s$ is the entropy. For ideal gas $\Gamma = (\gamma + 1)/2 > 1$. For some complex fluids and some particular conditions of pressure and temperature, $\Gamma$ may be lower that one, implying that $(\partial c/\partial \rho)_s < 0$. This means that the acceleration of pressure perturbations through a variable density fluids may be reversed and become a deceleration. It has been shown that, for $\Gamma << 1$, compression shocks are strongly reduced, thus alleviating the shock intensity. This has great potential in increasing the efficiency. This is why so much interest is put on dense gas ORCs.
The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [79]). The data to build these models is scarce due to the difficulty of performing reliable experiments. The related uncertainty is thus very high. Our work will go in the following directions:

1. develop deterministic models for the turbine and the other elements of the cycle. These will involve multi-dimensional high fidelity, as well as intermediate and low fidelity (one- and zero-dimensional), models for the turbine, and some 0D/1D models for other element of the cycle (pump, condenser, etc);

2. validation of the coupling between the various elements. The following aspects will be considered: characterization of the uncertainties on the cycle components (e.g. empirical coefficients modelling the pump or the condenser), calibration of the thermodynamic parameters, model the uncertainty of each element, and the influence of the unsteady experimental data;

3. demonstrate the interest of a specific optimization of geometry, operating conditions, and the choice of the fluid, according to the geographical location by including local solar radiation data. Multi-objective optimization will be considered to maximize performance indexes (e.g. Carnot efficiency, mechanical work and energy production), and to reduce the variability of the output.

This work will provide modern tools for the robust design of ORCs systems. It benefits from the direct collaboration with the SME EXOES (ANR LabCom VIPER), and from a collaboration with LEMMA.

Wave energy conversion is an emerging sector in energy engineering. The design of new and efficient Wave Energy Converters (WECs) is thus a crucial activity. As pointed out by Weber [143], it is more economical to raise the technology performance level (TPL) of a wave energy converter concept at low technology readiness level (TRL). Such a development path puts a greater demand on the numerical methods used. The findings of Weber also tell us that important design decisions as well as optimization should be performed as early in the development process as possible. However, as already mentioned, today the wave energy sector relies heavily on the use of tools based on simplified linear hydrodynamic models for the prediction of motions, loads, and power production. Our objective is to provide this sector, and especially SMEs, with robust design tools to minimize the uncertainties in predicted power production, loads, and costs of wave energy.

Following our initial work [91], we will develop, analyse, compare, and use for multi-fidelity optimization, non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisotropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [91], asymptotic models for WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

Once available, we will use this hierarchy of models to investigate and identify the modelling errors, and provide a more certain estimate of the cost of wave energy. Subsequently we will look into optimization cycles by comparing time-to-decision in a multi-fidelity optimization context. In particular, this task will include the development and implementation of appropriate surrogate models to reduce the computational cost of expensive high fidelity models. Here especially artificial neural networks (ANN) and Kriging response surfaces (KRS) will be investigated. This activity on asymptotic non-linear modelling for WECs, which has had very little attention in the past, will provide entirely new tools for this application. Multi-fidelity robust optimization is also an approach which has never been applied to WECs.

This work is the core of the EU OCEANErnanet MIDWEST project, which we coordinate. It will be performed in collaboration with our European partners, and with a close supervision of European SMEs in the sector, which are part of the steering board of MIDWEST (WaveDragon, Waves4Power, Tecnalia).
4.4. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [123].

The behaviour of a fibre bundle is actually extremely variable, as the oxidation reactions generating the self-healing mechanism have kinetics strongly dependent on temperature and composition. In particular, the lifetime of SH-CMCs depends on: (i) temperature and composition of the surrounding atmosphere; (ii) composition and topology of the matrix layers; (iii) the competition of the multidimensional diffusion/oxidation/volatilization processes; (iv) the multidimensional flow of the oxide in the crack; (v) the inner topology of fibre bundles; (vi) the distribution of critical defects in the fibres. Unfortunately, experimental investigations on the full materials are too long (they can last years) and their output too qualitative (the coupled effects can only be observed a-posteriori on a broken sample). Modelling is thus essential to study and to design SH-CMCs.

In collaboration with the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation to the transport equations (Fick’s laws) with chemical reactions sources, plus a potential model for the flow of oxide [82], [89], [121]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (see e.g. [78]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.5. Coastal and civil engineering

Our objective is to bridge the gap between the development of high order adaptive methods, which has mainly been performed in the industrial context and environmental applications, with particular attention to coastal and hydraulic engineering. We want to provide tools for adaptive non-linear modelling at large and intermediate scales (near shore, estuarine and river hydrodynamics). We will develop multi-scale adaptive models for free surface hydrodynamics. Beside the models and codes themselves, based on the most advanced numerics we will develop during this project, we want to provide sufficient know how to control, adapt and optimize these tools.

We will focus our effort in the understanding of the interactions between asymptotic approximations and numerical approximations. This is extremely important in at least two aspects. The first is the capability of a numerical model to handle highly dispersive wave propagation. This is usually done by high accuracy asymptotic PDE expansions. Here we plan to make heavily use of our results concerning the relations between...
vertical asymptotic expansions and standard finite element approximations. In particular, we will invest some effort in the development of $xy+z$ adaptive finite element approximations of the incompressible Euler equations. Local $p-$adaptation of the vertical approximation may provide a “variable depth” approximation exploiting numerics instead of analytical asymptotics to control the physical behaviour of the model.

Another important aspect which is not understood well enough at the moment is the role of dissipation in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [103], [127], [118], [86], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [136], [137], [135], [101], [93]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigated, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow some understanding of this interaction and to possibly propose considerably improved numerical methods [66].

5. Highlights of the Year

5.1. Highlights of the Year

- CARDAMOM has passed with success its first evaluation in March 2017
- The associated team HAMSTER between CARDAMOM and the Department of Civil engineering of Duke University has been created in January 2017
- The associated team COMMUNES between CARDAMOM and the CWI in the Netherlands has been created in January 2017
- The open-source consortium around the Mmg platform has been created, and Mmg will now be part of the projects managed by Inria Soft

6. New Software and Platforms

6.1. AeroSol

**Keyword:** Finite element modelling  
**Functional description:** The AeroSol software is a high order finite element library written in C++. The code has been designed so as to allow for efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The work of the team CARDAMOM (previously Bacchus) is focused on continuous finite elements methods, while the team Cagire is focused on discontinuous Galerkin methods. However, everything is done for sharing the largest part of code we can. More precisely, classes concerning IO, finite elements, quadrature, geometry, time iteration, linear solver, models and interface with PaMPA are used by both of the teams. This modularity is achieved by mean of template abstraction for keeping good performances. The distribution of the unknowns is made with the software PaMPA, developed within the team TADAAM (and previously in Bacchus) and the team Castor.  
**News of the year:** The following points have been developed in the code

*A postprocessing in the high order GMSH format has been added*
*On the Uhaina part, the work has been focused on the entropy viscosity approach for shock limiting, and on the positivity preserving limiters for ensuring positive water height.

*On the dealing of low Mach problems - Multidimensional numerical flux accurate for the computation of steady and unsteady low Mach flows. - Test cases at low Mach.

*A method for penalizing rigid bodies instead of meshing it has been developed within the postdoc of Marco Lorini. The model was implemented, an improvement of time schemes for steady problems was done. The method has been tested with 2d and 3d tests: bump, flow around a cylinder. These tests allowed to fix bugs, especially for wall boundary conditions. The coupling with adaptation tools has began.

*The library has benefited from the HPCLib Inria Hub, which aims at improving the development environment of HPC libraries within the Bordeaux Sud Ouest Centre. Within this project, a static analysis of the library based on sonarqube has been performed.

*A wiki for gathering the documentation of the different test cases has began.

- Participants: Benjamin Lux, Damien Genet, Dragan Amenga Mbengoue, Hamza Belkhayat Zougari, Mario Ricchiuto, Maxime Mogé, Simon Delmas and Vincent Perrier
- Contact: Vincent Perrier

### 6.2. Crysa

**KEYWORDS**: Image analysis - 2D

**FUNCTIONAL DESCRIPTION**: Analyzes the organization of objects placed in a hexagonal grid in an image and the crystalline structure induced in this image.

- Participants: Cécile Dobrzynski and Jean Mercat
- Partners: LCTS (UMR 5801) - LCPO - ISM
- Contact: Cécile Dobrzynski

### 6.3. Cut-ANOVA

**Cut-ANOVA Global Sensitivity Analysis**

**KEYWORDS**: Stochastic models - Uncertainty quantification

**SCIENTIFIC DESCRIPTION**: An anchored analysis of variance (ANOVA) method is proposed to decompose the statistical moments. Compared to the standard ANOVA with mutually orthogonal component functions, the anchored ANOVA, with an arbitrary choice of the anchor point, loses the orthogonality if employing the same measure. However, an advantage of the anchored ANOVA consists in the considerably reduced number of deterministic solver’s computations, which renders the uncertainty quantification of real engineering problems much easier. Different from existing methods, the covariance decomposition of the output variance is used in this work to take account of the interactions between non-orthogonal components, yielding an exact variance expansion and thus, with a suitable numerical integration method, provides a strategy that converges. This convergence is verified by studying academic tests. In particular, the sensitivity problem of existing methods to the choice of anchor point is analyzed via the Ishigami case, and we point out that covariance decomposition survives from this issue. Also, with a truncated anchored ANOVA expansion, numerical results prove that the proposed approach is less sensitive to the anchor point. The covariance-based sensitivity indices (SI) are also used, compared to the variance-based SI. Furthermore, we emphasize that the covariance decomposition can be generalized in a straightforward way to decompose higher-order moments. For academic problems, results show the method converges to exact solution regarding both the skewness and kurtosis. The proposed method can indeed be applied to a large number of engineering problems.
FUNCTIONAL DESCRIPTION: The Cut-ANOVA code (Fortran 90, MPI + OpenMP) is devoted to the stochastic analysis of numerical simulations. The method implemented is based on the spectral expansion of "anchored ANOVA", allowing the covariance-based sensitivity analysis. Compared to the conventional Sobol method, "Cut-ANOVA" provides three sensitivity indices instead of one, which allows a better analysis of the reliability of the numerical prediction. On the other hand, "Cut-ANOVA" is able to compute the higher order statistical moments such as the Skewness (3-rd order moment) and Kurtosis (4-th order moment). Several dimension reduction techniques have also been implemented to reduce the computational cost. Finally, thanks to the innovative method implemented into the Code Cut-ANOVA, one can obtain a similar accuracy for stochastic quantities by using a considerably less number of deterministic model evaluations, compared with the classical Monte Carlo method.

- Participants: Kunkun Tang and Pietro-Marco Congedo
- Contact: Kunkun Tang

6.4. Fmg

KEYWORD: Mesh adaptation

FUNCTIONAL DESCRIPTION: FMG is a library deforming an input/reference simplicial mesh w.r.t. a given smoothness error monitor (function gradient or Hessian), metric field, or given mesh size distribution. Displacements are computed by solving an elliptic Laplacian type equation with a continuous finite element method. The library returns an adapted mesh with a corresponding projected solution, obtained by either a second order projection, or by an ALE finite element remap. The addiction of a new mass conservative approach developed ad-hoc for shallow water flows is under way.

NEWS OF THE YEAR: - Development of the Elasticity model to compute the nodes displacement. - Development of a new model to compute the nodes displacement. This mixed model takes the advantages of the Laplacian model and the Elasticity model: a refined mesh where the solution varies a lot and a smooth gradation of the edges size elsewhere. - Extension in three dimension

- Participants: Cécile Dobrzynski, Leo Nouveau, Luca Arpaia and Mario Ricchiuto
- Contact: Cécile Dobrzynski

6.5. Mmg

Mmg Platform

KEYWORDS: Mesh adaptation - Anisotropic - Mesh generation - Mesh - Isovalue discretization

SCIENTIFIC DESCRIPTION: The Mmg plateform gathers open source software for two-dimensional, surface and volume remeshing. The platform software perform local mesh modifications. The mesh is iteratively modified until the user prescriptions satisfaction.

The 3 softwares can be used by command line or using the library version (C, C++ and Fortran API) : - Mmg2d performs mesh generation and isotropic and anisotropic mesh adaptation. - Mmgs allows isotropic and anisotropic mesh adaptation for 3D surface meshes. - Mmg3d is a new version of the MMG3D4 software. It remesh both the volume and surface mesh of a tetrahedral mesh. It performs isotropic and anisotropic mesh adaptation and isovalue discretization of a level-set function. The platform software allow to control the boundaries approximation: The "ideal" geometry is reconstruct from the piecewise linear mesh using cubic Bezier triangular partches. The surface mesh is modified to respect a maximal Hausdorff distance between the ideal geometry and the mesh.

Inside the volume, the software perform local mesh modifications ( such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).

FUNCTIONAL DESCRIPTION: The Mmg platform gathers open source software for two-dimensional, surface and volume remeshing. It provides three applications : 1) mmg2d: generation of a triangular mesh , adaptation and optimization of a triangular mesh 2) mmgs: adaptation and optimization of a surface triangulation representing a piecewise linear approximation of an underlying surface geometry 3) mmg3d: adaptation and optimization of a tetrahedral mesh and isovalue discretization
The platform software perform local mesh modifications. The mesh is iteratively modified until the user prescription satisfaction.

**NEWS OF THE YEAR:** Release 5.3.0 improves: - the mmg3d algorithm for mesh adaptation (better convergence and edge lengths closest to 1) - the software behaviour in case of failure (warnings/error messages are printed only 1 time and there is no more exits in the code) - the mmg2d software that now uses the same structure than mmgs and mmg3d

It adds: - the -hsiz option for mmg2d/s/3d (that allows to generate a uniform mesh of size ) - the -nosurf option for mmg2d (that allows to not modify the mesh boundaries) - the -opnbdy option for mmg3d (that allow to preserve an open boundary inside a volume mesh) - the possibility to provide meshes containing prisms to mmg3d (the prisms entities are preserved while the tetra ones are modified)

- Participants: Algiane Froehly, Cécile Dobrzynski, Charles Dapogny and Pascal Frey
- Partners: Université de Bordeaux - CNRS - IPB - UPMC
- Contact: Cécile Dobrzynski
- URL: http://www.mmgtools.org

### 6.6. MMG3D

**Mmg3d**

**KEYWORDS:** Mesh - Anisotropic - Mesh adaptation

**SCIENTIFIC DESCRIPTION:** Mmg3d is an open source software for tetrahedral remeshing. It performs local mesh modifications. The mesh is iteratively modified until the user prescriptions satisfaction.

Mmg3d can be used by command line or using the library version (C, C++ and Fortran API) : - It is a new version af the MMG3D4 software. It remesh both the volume and surface mesh of a tetrahedral mesh. It performs isotropic and anisotropic mesh adaptation and isovalue discretization of a level-set function.

Mmg3d allows to control the boundaries approximation: The "ideal" geometry is reconstruct from the piecewise linear mesh using cubic Bezier triangular patches. The surface mesh is modified to respect a maximal Hausdorff distance between the ideal geometry and the mesh.

Inside the volume, the software perform local mesh modifications ( such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).

**FUNCTIONAL DESCRIPTION:** Mmg3d is one of the software of the Mmg platform. Is is dedicated to the modification of 3D volume meshes. It perform the adaptation and the optimization of a tetrahedral mesh and allow to discretize an isovalue.

Mmg3d perform local mesh modifications. The mesh is iteratively modified until the user prescription satisfaction.

- Participants: Algiane Froehly, Cécile Dobrzynski, Charles Dapogny and Pascal Frey
- Partners: Université de Bordeaux - CNRS - IPB - UPMC
- Contact: Cécile Dobrzynski
- URL: http://www.mmgtools.org

### 6.7. NOMESH

**KEYWORDS:** Mesh - Curved mesh - Tetrahedral mesh

**FUNCTIONAL DESCRIPTION:** NOMESH is a software allowing the generation of three order curved simplicial meshes. Starting from a "classical" mesh with straight elements composed by triangles and/or tetrahedra, we are able to curve the boundary mesh. Starting from a mesh with some curved elements, we can verify if the mesh is valid, that means there is no crossing elements and only positive jacobian. If the curved mesh is non valid, we modify it using linear elasticity equations until having a valid curved mesh.

- Participants: Algiane Froehly, Ghina El Jannoun and Cécile Dobrzynski
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Cécile Dobrzynski
6.8. ORComp

**FUNCTIONAL DESCRIPTION:** The ORComp platform is a simulation tool permitting to design an ORC cycle. Starting from the solar radiation, this platform computes the cycle providing the best performance with optimal choices of the fluid and the operating conditions. It includes RobUQ, a simulation block of the ORC cycles, the RealfluiDS code for the simulation of the turbine and of the heat exchanger, the software FluidProp (developed at the University of Delft) for computing the fluid thermodynamic properties.

- **Participants:** Maria-Giovanna Rodio and Pietro-Marco Congedo
- **Contact:** Maria-Giovanna Rodio
- **URL:** [https://github.com/Orcomp/Orcomp](https://github.com/Orcomp/Orcomp)

6.9. RealfluiDS

**KEYWORDS:** Compressible flows - Finite element modelling - Residual distribution - Aeronautics

**FUNCTIONAL DESCRIPTION:** RealfluiDS is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multimaterial, MHD flows and turbulent flows (using the SA model). There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in the 3D one. This software implements the more recent residual distribution schemes. The code has been parallelized with and without overlap of the domains. The uncertainty quantification library RobUQ has been coupled to the software. A partitioning tool exists in the package, which uses Scotch. Recently, the code has been developed for taking into account real-gas effects, in order to use arbitrarily complex equations of state. Further developments concerning multiphase effects are under way.

- **Participants:** Cécile Dobrzynski, Héloïse Beaugendre, Leo Nouveau, Pietro-Marco Congedo and Quentin Viville
- **Contact:** Héloïse Beaugendre

6.10. SH-COMP

**KEYWORDS:** Finite element modelling - Multi-physics simulation - Chemistry - Incompressible flows - 2D

**FUNCTIONAL DESCRIPTION:** Numerical modelling of the healing process in ceramic matrix composites

- **Participants:** Gérard Vignoles, Gregory Perrot, Guillaume Couegnat, Mario Ricchiuto and Virginie Drean
- **Partner:** LCTS (UMR 5801)
- **Contact:** Guillaume Couegnat

6.11. SLOWS

*Shallow-water fLows*

**KEYWORDS:** Simulation - Free surface flows - Unstructured meshes

**SCIENTIFIC DESCRIPTION:** Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach. Newton and frozen Newton loops are used to solve the implicit nonlinear equations. The linear algebraic systems arising in the discretization are solved with the MUMPS library. This year implicit and explicit (extrapolated) multistep higher order time integration methods have been implemented, and a mesh adaptation technique based on simple mesh deformation has been also included.

**FUNCTIONAL DESCRIPTION:** SLOWS is a C-platform allowing the simulation of free surface shallow water flows with friction. It can be used to simulate near shore hydrodynamics, wave transformations processes, etc.

- **Participants:** Andrea Filippini, Luca Arpaia, Maria Kazolea, Mario Ricchiuto and Nikolaos Pattakos
- **Contact:** Mario Ricchiuto
6.12. Sparse-PDD

Adaptive sparse polynomial dimensional decomposition for global sensitivity analysis

**Keywords:** Stochastic models - Uncertainty quantification

**Scientific Description:** The polynomial dimensional decomposition (PDD) is employed in this code for the global sensitivity analysis and uncertainty quantification (UQ) of stochastic systems subject to a moderate to large number of input random variables. Due to the intimate structure between the PDD and the Analysis of Variance (ANOVA) approach, PDD is able to provide a simpler and more direct evaluation of the Sobol’ sensitivity indices, when compared to the Polynomial Chaos expansion (PC). Unfortunately, the number of PDD terms grows exponentially with respect to the size of the input random vector, which makes the computational cost of standard methods unaffordable for real engineering applications. In order to address the problem of the curse of dimensionality, this code proposes essentially variance-based adaptive strategies aiming to build a cheap meta-model (i.e. surrogate model) by employing the sparse PDD approach with its coefficients computed by regression. Three levels of adaptivity are carried out in this code: 1) the truncated dimensionality for ANOVA component functions, 2) the active dimension technique especially for second- and higher-order parameter interactions, and 3) the stepwise regression approach designed to retain only the most influential polynomials in the PDD expansion. During this adaptive procedure featuring stepwise regressions, the surrogate model representation keeps containing few terms, so that the cost to resolve repeatedly the linear systems of the least-square regression problem is negligible. The size of the finally obtained sparse PDD representation is much smaller than the one of the full expansion, since only significant terms are eventually retained. Consequently, a much less number of calls to the deterministic model is required to compute the final PDD coefficients.

**Functional Description:** This code allows an efficient meta-modeling for a complex numerical system featuring a moderate-to-large number of uncertain parameters. This innovative approach involves polynomial representations combined with the Analysis of Variance decomposition, with the objective to quantify the numerical output uncertainty and its sensitivity upon the variability of input parameters.

- **Participants:** Kunkun Tang and Pietro-Marco Congedo
- **Contact:** Kunkun Tang

6.13. TUCWave

**Keyword:** Physical simulation

**Scientific Description:** A novel work that advances a step ahead the methodology of the solution of dispersive models. TUCWave uses a high-order well-balanced unstructured finite volume (FV) scheme on triangular meshes for modeling weakly nonlinear and weakly dispersive water waves over varying bathymetries, as described by the 2D depth-integrated extended Boussinesq equations of Nwogu (1993), rewritten in conservation law form. The FV scheme numerically solves the conservative form of the equations following the median dual node-centered approach, for both the advective and dispersive part of the equations. The code developed follows an efficient edge based structured technique. For the advective fluxes, the scheme utilizes an approximate Riemann solver along with a well-balanced topography source term up-winding. Higher order accuracy in space and time is achieved through a MUSCL-type reconstruction technique and through a strong stability preserving explicit Runge-Kutta time stepping. Special attention is given to the accurate numerical treatment of moving wet/dry fronts and boundary conditions. Furthermore, the model is applied to several examples of wave propagation over variable topographies and the computed solutions are compared to experimental data.

**Functional Description:** Fortran Planform which accounts for the study of near shore processes

- **Participants:** Argiris Delis, Ioannis Nikolos and Maria Kazolea
- **Partner:** CNRS
- **Contact:** Maria Kazolea
7. New Results

7.1. High order discretizations on unstructured meshes

- Participants: Héloïse Beaugendre, Cécile Dobrzynski, Mario Ricchiuto, Quentin Viville
- Corresponding member: Héloïse Beaugendre

A \( p \)-adaptive continuous residual distribution scheme has been proposed. Under certain conditions, primarily the expression of the total residual on a given element \( K \) into residuals on the sub-elements of \( K \) and the use of a suitable combination of quadrature formulas, it is possible to change locally the degree of the polynomial approximation of the solution. The discrete solution can then be considered non continuous across the interface of elements of different orders, while the numerical scheme still verifies the hypothesis of the discrete Lax–Wendroff theorem which ensures its convergence to a correct weak solution. The construction of our \( p \)-adaptive method has been done in the frame of a continuous residual distribution (RD) scheme. Different test cases for non-linear equations at different flow velocities demonstrate numerically the validity of the theoretical results.

As an evolution, a \( hp \)-adaptive RD scheme for the penalized Navier-Stokes equations has also been developed. The method combines \( hp \)-adaptation and penalization within a Residual Distribution scheme. The proposed method is an embedded boundary method that provides a simple and accurate treatment of the wall boundary conditions by the technique of penalization and anisotropic mesh adaptation. This method extends the IBM-LS-AUM method to higher order elements and is based on the construction of a \( p \)-adaptive RD scheme combined with an anisotropic mesh adaptation method. It has been applied to the resolution of the penalized Navier-Stokes equations. The robustness of the method is showed in practice with numerical experiments for different Mach regimes and Reynolds numbers in dimension two and three.

A novel formulation of residual distributions schemes as well as finite volume schemes on unstructured triangulations in curvilinear coordinates has been proposed within the PhD of L. Arpaia [31], generalising the work of [3]. The simulations reveal that the RD method proposed has very low dissipation when compared to the results existing in literature. This is very encouraging for applications in meteorology. A positivity preserving variant of the method has been used to compute large scale impact and inundation of the 2011 Tohoku tsunami [33], [32].

7.2. High order mesh generation and mesh adaptation

- Participants: Luca Arpaia, Cécile Dobrzynski, Marco Lorini, Mario Ricchiuto
- Corresponding member: Cécile Dobrzynski

This year several new algorithmic improvements have been obtained which will allow to enhance our meshing tools:

- We have enhanced our work on \( r \)-adaptation techniques for time dependent equations. These techniques are based on mesh deformations obtained by solving continuous differential equations for the local displacements. These equations are controlled by an error monitor. Several improvements have been made. We have proposed a new mixed model to compute the mesh deformations. This model is based on one hand on a Laplacian model and on the other hand on an Elasticity model. It takes advantages of the two approaches: a refined mesh where the solution varies a lot and a smooth gradation of the edges size elsewhere. We have applied this technic to 2d unsteady compressible simulations and we have preliminary results in three dimensions.

- Additional work on \( r \)-adaptation has also involved a simple extension to spherical coordinates, allowing an efficient treatment of inundation caused by large scale tsunami waves [33], [32].
A novel strategy to solve the finite volume discretization of the unsteady Euler equations within the ALE framework over tetrahedral adaptive grids have been proposed [11]. The volume changes due to local mesh adaptation are treated as continuous deformations of the finite volumes and they are taken into account by adding fictitious numerical fluxes to the governing equation. This peculiar interpretation enables to avoid any explicit interpolation of the solution between different grids and to compute grid velocities so that the GCL is automatically fulfilled also for connectivity changes. The solution on the new grid is obtained through standard ALE techniques, thus preserving the underlying scheme properties, such as conservativeness, stability and monotonicity. The adaptation procedure includes node insertion, node deletion, edge swapping and points relocation and it is exploited both to enhance grid quality after the boundary movement and to modify the grid spacing to increase solution accuracy. We have demonstrated the ability of the method on three-dimensional simulations of steady and unsteady flow fields.

We extended our technique for generating high order curved meshes to immersed boundary problem. Based on a level-set function, we curved the mesh according to the 0-level-set. Preliminary results in 2d have been performed for compressible simulations.

Initial work on the use of fitting techniques to exactly compute moving shocks has been performed. The benefit of this approach in completely removing all numerical artefacts related to the capturing of the discontinuity, and in recovering the full order of accuracy have been shown for both straight and mildly curved discontinuities [42].

7.3. Uncertainty Quantification and robust design optimization

Participants: Andrea Cortesi, Pietro Marco Congedo, Nassim Razaaly, Sanson Francois
Corresponding member: Pietro Marco Congedo

Concerning Uncertainty Quantification techniques, we have worked in three main directions. First, we developed novel techniques for building efficient and low-cost surrogate. In [43], two main points are introduced. Firstly, a technique which couples Universal Kriging with sparse Polynomial Dimensional Decomposition (PDD) to build a metamodel with improved accuracy. The polynomials selected by the adaptive PDD representation are used as a sparse basis to build an Universal Kriging surrogate model. The second is a strategy, derived from anisotropic mesh adaptation, to adaptively add a fixed number of new training points to an existing Design of Experiments. Moreover, we have explored in [44] how active subspaces are used to find a low-dimensional dependence structures in the input-to-output map of the forward numerical solver. Then, surrogate models on the active variables are used to accelerate the forward uncertainty propagation by Monte Carlo sampling and the Markov Chain Monte Carlo sampling of the posterior distribution for Bayesian inversion. Then, the forward and backward methodologies are applied to the simulation of a hypersonic flow around a cylinder, in conditions for which experimental data are available, revealing new insights towards the potential exploitation of heat flux data for freestream rebuilding.

The second action has been oriented towards the development of efficient techniques for computing low-probability estimations. In [50], we have proposed a novel algorithm permitting to both building an accurate metamodel and to provide a statistically consistent error. In fact, it relies on a novel metamodel building strategy, which aims to refine the limit-state region in all the branches "equally", even in the case of multiple failure regions, with a robust stopping building criterion. Additionally, another importance sampling technique is proposed, permitting to drastically reduce the computational cost when estimating some reference values, or when a very weak failure-probability event should be computed directly from the metamodel.

Third, we have worked on the propagation of uncertainties through systems of solvers [25]. A System of Solvers (SoS) is a set of interdependent solvers where an output of an upstream solver can be the input of downstream solvers. In this work, we restrict ourselves to directed SoS with one-way dependences between solvers. Performing Uncertainty Quantification (UQ) analysis in SoS is challenging because it typically encapsulates a large number of uncertain input parameters and classical UQ methods, such as spectral expansions and Gaussian process models, are affected by the curse of dimensionality. In this work, we develop
an original mathematical framework, based on Gaussian Process (GP) models to construct a global surrogate model of the uncertain SoS, that can be used to solve forward and backward UQ problems. The key idea of the proposed approach is to determine a local GP model for each solver constituting the SoS. These local GP models are built adaptively to satisfy criteria based on the global output error estimation. The error estimate can be decomposed into contributions from the individual GP models, enabling one to select the GP models to refine to efficiently reduce the global error. The framework is first tested on several analytical problems and subsequently applied to space object reentry simulations.

Concerning optimization under uncertainties, we have worked on the formulation of novel framework to perform multi-objective optimization [24], when considering an error on the objective functions. In many engineering optimization problems, the objective functions are affected by an error arising from the model employed for the computation of the functions. For example, in the case of uncertainty-based optimization the objective functions are statistics of a performance of interest which is uncertain due to the variability of the system input variables. These estimated objectives are affected by an error, which can be modeled with a confidence interval. The framework proposed here is general and aims at dealing with any error affecting a given objective function. The strategy is based on the extension of the Bounding-Box concept to the Pareto optima, where the error can be regarded with the abstraction of an interval (in one-dimensional problems) or a Bounding-Box (in multi-dimensional problems) around the estimated value. This allows the computation of an approximated Pareto front, whose accuracy is strongly dependent on the acceptable computational cost. This approach is then supplemented by the construction of an evolutive surrogate model on the objective functions, iteratively refined during the optimization process. This allows ultimately to further reduce the computation cost of the Pareto front with approximations of the objective functions at a negligible cost. Regarding optimization, we have also worked on the formulation of a novel optimization under uncertainty framework for the definition of optimal shapes for morphing airfoils, applied here to advancing/retreating 2D airfoils. In particular, the morphing strategy is conceived with the intent of changing the shape at a given frequency to enhance aerodynamic performance. The optimization of morphing airfoils pre- sented here only takes into account the aerodynamic performance. The paper [5] is then focused on an aerodynamic optimization to set the optimal shape with respect to performance, where technological aspects are inserted through geometrical constraints.

7.4. Modelling of free surface flows

- Participants: Luca Arpaia, Mathieu Colin, Andrea Filippini, Maria Kazolea, Luc Mieussens, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

This year we continue our work on fully non-linear weakly dispersive wave models in two dimensional horizontal coordinates. The proposed framework in [92], to approximate the so-called 2D Green-Naghdi equations has been presented in ISOPE (citation) conference an new paper is under preparation.

We also continue our study on wave breaking techniques on BT models [48]. We studied weakly and fully nonlinear models representative of classical and well known models/codes such as BOUSS-2D [85], [86], Funwave [144], [129], Coulwave [109], [131], BOSZ [128], MIKE21 [83], TUCWave [100], [101], and others. We have in particular focused on the enhanced equations of Nwogu [117], and on a frequency enhanced version of the Green-Naghdi system in the form proposed in [69], [93]. We have compared the now popular hybrid closure initially proposed in [136], with an eddy viscosity closure based on an adaptation of the turbulent kinetic energy closure model of [118], modified to be consistent with the detection mechanisms proposed of [101], [93], and also used here. The study performed has involved: a systematic analysis of the behaviour of the two closures for different mesh sizes; the use of dissipation monitors, consistent with the available theory of entropy dissipation for conservation laws [132], [133], to study the dynamics of breaking for several cases; thorough evidence of the equivalent capabilities of the two approaches to provide satisfactory results. Our results indicate that indeed, at least with the (rather standard) implementation proposed here, both closure approaches allow to describe correctly wave transformation and breaking at large scales. We have shown that when using the TKE eddy viscosity closure the numerical dissipation plays a negligible role, which motivates
to look for non-dissipative/energy conserving numerical methods in the future. Also, the results clearly show the reduced sensitivity to the mesh of this approach compared to the hybrid one. The analysis of the wave breaking of solitary waves on a slope also has allowed to quantitatively study the interplay of the dissipation introduced by friction, eddy viscosity, and numerical dissipation. A research paper is under review.

Further more we continue our work for weakly non linear weakly dispersive models, on the transformation breaking and run-up of irregular waves. Its is the first time that an unstructured high-resolution FV numerical solver for the 2D extended BT equations of Nwogu is tested on the generation and propagation of irregular waves. A research paper is under review.

The tools developed have been also used intensively in funded research programs. Within the TANDEM project, several benchmarks relevant to tsunami modelling have been performed and several common publications with the project partners are submitted and/or in preparation [6], [140]. We also our code SLOWS, to study the conditions for tidal bore formation in convergent alluvial estuaries [70]. A new set of dimensionless parameters has been introduced to describe the problem, and the code SLOWS has been used to explore the space of these parameters allowing to determine a critical curve allowing to characterize an estuary as "bore forming" or not. Surprising physical behaviours, in terms of dissipation and nonlinearity of the tides, have been highlighted.

7.5. Wave energy conversion hydrodynamics

- Participants: Umberto Bosi, Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

We have proposed an efficient nonlinear modelling tool for the analysis of wave body interaction based on Boussinesq-type equations. The approach develop here is based on a PDE formulation which model the flow under the body with a depth averaged system featuring an unknown pressure for which a Poisson type problem must solved by appropriately embedding the constraint on the position of the body. The PDE system is discretised by means of a high-order continuous spectral/hp element method in which the coupling between the free surface and floater domains is handled by means of numerical fluxes inspired by techniques used in the discontinuous Galerkin approach. The model is now fully validated both in the hydrostatic case and in the non-hydrostatic one [36], [37]. Several extensions are under way within the MIDWEST project.

7.6. Kinetic modelling of rarefied gases and space reentry

- Participants: Giorgio Martalò, Luc Mieussens, Julien Mathiaud
- Corresponding member: Luc Mieussens

After the end of the post-doc of Giorgio Martalò, a paper has been published [2], in which as presented the derivation of modified boundary conditions for the compressible Navier-Stokes equations to take into account rarefied flow effects. Another paper, related to some numerical aspects, should be submitted soon. Moreover, a paper written by J. Mathiaud and L. Mieussens [7]. This is an extension of their previous work on the modelling of collisions in gases by Fokker-Planck model to polyatomic gases.

Finally, Baranger et. al [53] have presented a way to obtain correct numerical boundary conditions for the approximation of the Boltzmann equation to take into account collisions of gas molecules with solid boundaries. Standard second order finite volume schemes degenerate to first order close to solid walls, but it has been shown in [53] that a suitable use of extrapolation and slope limiters can give second order accuracy. This greatly improves the computation of the heat flux on solid boundaries for atmospheric re-entry flow simulation, for instance.

Finally, the project of numerical and physical modelling of the liquid ablation (for atmospheric re-entry flows) has been concluded by the defense of Simon Peluchon in November 2017. So far, one paper has been published on this subject [8], but at least another one should be submitted soon. Note that Simon Peluchon will be hired in the CEA as a researcher-engineer in January 2018. This subject might induce new collaborations between the CEA and Cardamom, in particular for the use of unstructured grids.
We have developed some activities concerning the application of UQ analysis to aerospace problems. First, we have illustrated in [44] how to perform a Bayesian calibration of the free stream parameters of a hypersonic high-enthalpy flow around a cylinder, exploiting active subspaces for the reduction of the dimensionality of the input space. The configuration taken into account was the HEG I configuration, known in literature as a validation test-case for hypersonic CFD. The goal of the Bayesian inversion was to show the feasibility in using measurements of pressure and heat flux at the stagnation point for rebuilding freestream velocity and density.

Then, we have realized several studies concerning ablation and the characterization of ablative materials. In particular, in [16] and [15], we have illustrated a proof-of-concept of the coupling between a thermo-chemical ablation model and modern uncertainty quantification techniques with the aim of rebuilding the ablative material tests performed in the inductively coupled Plasmatron facility at the von Karman Institute. Finally, in [14], we have shown how an approach that uses uncertainty quantification methodology can be used in order to rigorously compute error bars on numerically rebuilt values of enthalpy and catalycity from the Plasmatron facility.

7.7. Modelling of icing/de-icing

- Participants: Héloïse Beaugendre, Léo Nouveau, Cécile Dobrzynski and Mario Ricchiuto
- Corresponding member: Héloïse Beaugendre

The final public workshop of the European STORM project took place at the end of March 2017. The novel high-fidelity approach, based on penalization, proposed by Cardamom to model ice block trajectories has been compared to a low-fidelity approach from Airbus, to two chimera grids approaches from DLR and ONERA and to an experimental database elaborated during the project. The preliminary results are encouraging and commit to further developments of the method.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- THALES, Activity around the numerical certification of debris codes, Coordinator: P.M. Congedo, 23 Keuros;
- ArianeGroup, Activity around techniques for computing low-probabilities, Coordinator: P.M. Congedo, 20 Keuros;
- CEA-CESTA, Coordinator: P.M. Congedo, 40 Keuros;
- An open-source consortium have been created around the Mmg platform. There are 3 members for 2017:
  - SAFRAN Tech, silver member, 20 Keuros;
  - “Environnement des codes” laboratory, CEA-Cesta, silver member, 3 Keuros;
  - Coria laboratory, INSA Rouen, silver member, 3 Keuros.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR MAIDESC

Title: Maillages adaptatifs pour les interfaces instationnaires avec deformations, etirements, courbures.
Project-Team CARDAMOM

Type: ANR
Duration: 48 months
Starting date: 1st Oct 2013
Coordinator: Dervieux Alain (Inria Sophia)

Abstract: Mesh adaptive numerical methods allow computations which are otherwise impossible due to the computational resources required. We address in the proposed research several well identified main obstacles in order to maintain a high-order convergence for unsteady Computational Mechanics involving moving interfaces separating and coupling continuous media. A priori and a posteriori error analysis of Partial Differential Equations on static and moving meshes will be developed from interpolation error, goal-oriented error, and norm-oriented error. From the minimization of the chosen error, an optimal unsteady metric is defined. The optimal metric is then converted into a sequence of anisotropic unstructured adapted meshes by means of mesh regeneration, deformation, high stretching, and curvature. A particular effort will be devoted to build an accurate representation of physical phenomena involving curved boundaries and interfaces. In association with curved boundaries, a part of studies will address third-order accurate mesh adaption. Mesh optimality produces a nonlinear system coupling the physical fields (velocities, etc.) and the geometrical ones (unsteady metric, including mesh motion). Parallel solution algorithms for the implicit coupling of these different fields will be developed. Addressing efficiently these issues is a compulsory condition for the simulation of a number of challenging physical phenomena related to industrial unsolved or insufficiently solved problems. Non-trivial benchmark tests will be shared by consortium partners and by external attendees to workshops organized by the consortium. The various advances will be used by SME partners and proposed in software market.

9.1.2. PIA TANDEM

Title: Tsunamis in the Atlantic and the English Channel: Definition of the Effects through numerical Modeling (TANDEM)
Type: PIA - RSNR (Investissement d’Avenir, "Recherches en matière de Sûreté Nucléaire et Radioprotection")
Duration: 48 months
Starting date: 1st Jan 2014
Coordinator: H. Hebert (CEA)

Abstract: TANDEM is a project dedicated to the appraisal of coastal effects due to tsunami waves on the French coastlines, with a special focus on the Atlantic and Channel coastlines, where French civil nuclear facilities have been operated since about 30 years. As identified in the call RSNR, this project aims at drawing conclusions from the 2011 catastrophic tsunami, in the sense that it will allow, together with a Japanese research partner, to design, adapt and check numerical methods of tsunami hazard assessment, against the outstanding observation database of the 2011 tsunami. Then these validated methods will be applied to define, as accurately as possible, the tsunami hazard for the French Atlantic and Channel coastlines, in order to provide guidance for risk assessment on the nuclear facilities.

9.1.3. FUI ICARUS

Title: Intensive Calculation for AeRo and automotive engines Unsteady Simulations.
Type: FUI
Duration: January 2017 - December 2019
Coordinator: Turbomeca, Safran group

9.1.4. APP Bordeaux 1

Title: Reactive fluid flows with interface: macroscopic models and application to self-healing materials
Type : Project Bordeaux 1  
Duration : 36 months  
Starting : September 2014  
Coordinator : M. Colin  

Abstract : Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research, for aerospace and energy applications involving high temperatures. Though based on brittle ceramic components, these composites are not brittle due to the use of a fiber/matrix interphase that manages to preserve the fibers from cracks appearing in the matrix. The lifetime-determining part of the material is the fibers, which are sensitive to oxidation; when the composite is in use, it contains cracks that provide a path for oxidation. The obtained lifetimes can be of the order of hundreds of thousands of hours. These time spans make most experimental investigations impractical. In this direction, the aim of this project is to furnish predictions based on computer models that have to take into account: 1. the multidimensional topology of the composite made up of a woven ceramic fabric; 2. the complex chemistry taking place in the material cracks; 3. the flow of the healing oxide in the material cracks.

9.1.5. APP University of Bordeaux  
Title : Modélisation d’un système de dégivrage thermique  
Type : Project University of Bordeaux  
Duration : 36 months  
Starting : October 2016  
Coordinator : H. Beaugendre and M. Colin  

Abstract : From the beginning of aeronautics, icing has been classified as a serious issue : ice accretion on airplanes is due to the presence of supercooled droplets inside clouds and can lead to major risks such as aircrash for example. As a consequence, each airplane has its own protection system : the most important one is an anti-icing system which runs permanently. In order to reduce gas consumption, de-icing systems are developed by manufacturers. One alternative to real experiment consists in developing robust and reliable numerical models : this is the aim of this project. These new models have to take into account multi-physics and multi-scale environment : phase change, thermal transfer, aerodynamics flows, etc. We aim to use thin films equations coupled to level-set methods in order to describe the phase change of water. The overall objective is to provide a simulation platform, able to provide a complete design of these systems.

9.1.6. CRA - Region Aquitaine  
Title : Virtual prototyping of EVE engines  
Type : Co-funded from Region Aquitaine and Inria  
Duration : 36 months  
Starting : January 2017  
Coordinator : P.M. Congedo  

Abstract : The main objective of this thesis is the construction of a numerical platform, for permitting an efficient virtual prototyping of the EVE expander. This will provide EXOES with a numerical tool, that is much more predictive with respect to the tools currently available and used in EXOES, by respecting an optimal trade-off in terms of complexity/cost needed during an industrial design process. Two research axes will be mainly developed. First, the objective is to perform some high-predictive numerical simulation for reducing the amount of experiments, thanks to a specific development of RANS tools (Reynolds Averaged Navier-Stokes equations) for the fluids of interest for EXOES. These tools would rely on complex thermodynamic models and a turbulence model that should be modified. The second axis is focused on the integration of the solvers of different fidelity in a multi-fidelity platform for performing optimization under uncertainties. The idea is to evaluate the system performances by using massively the low-fidelity models, and by correcting these estimations via only few calculations with the high-fidelity code.
9.2. European Initiatives

9.2.1. Collaborations in European Programs, Except FP7 & H2020

Program: Ocean ERANET
Project acronym: MIDWEST
Project title: Multi-fidelity decision making tools for wave energy systems
Duration: October 2015- October 2018
Coordinator: M. Ricchiuto
Other partners: Chalmers University (Sweden), IST Lisbon (Portugal), DTU Compute (Denmark)
MIDWEST is a project starting in 2016 (kick-off in December 2015) and funded by the EU-OceaneraNET program by the French ADEME, by the Swedish SWEA, and by the Portuguese FCT, aiming at proposing new tools for the wave energy industry. Wave energy converters (WECs) design currently relies on low-fidelity linear hydrodynamic models. While these models disregard fundamental nonlinear and viscous effects – which might lead provide sub-optimal designs – high-fidelity fully nonlinear Navier-Stokes models are prohibitively computational expensive for optimization. The MIDWEST project will provide an efficient asymptotic nonlinear finite element model of intermediate fidelity, investigate the required fidelity level to resolve a given engineering output, construct a multi-fidelity optimization platform using surrogate models blending different fidelity models. Combining know how in wave energy technology, finite element modelling, high performance computing, and robust optimization, the MIDWEST project will provide a new efficient decision making framework for the design of the next generation WECs which will benefit all industrial actors of the European wave energy sector.

Program: H2020 MSCA-ITN
Project acronym: UTOPIAE
Project title: Handling the unknown at the edge of tomorrow
Duration: January 2017- December 2020
Coordinator: M. Vasile (Strathclyde University)
Other partners: see http://utopiae.eu/ for additional details
UTOPIAE is a European research and training network looking at cutting edge methods bridging optimisation and uncertainty quantification applied to aerospace systems. The network will run from 2017 to 2021, and is funded by the European Commission through the Marie Sklodowska-Curie Actions of H2020. The network is made up of 15 partners across 6 European countries, including the UK, and one international partner in the USA, collecting mathematicians, engineers and computer scientists from academia, industry, public and private sectors.
Mission statement : To train, by research and by example, 15 Early Stage Researchers in the field of uncertainty quantification and optimisation to become leading independent researchers and entrepreneurs that will increase the innovation capacity of the EU. To equip the researchers with the skills they will need for successful careers in academia and industry. To develop fundamental mathematical methods and algorithms to bridge the gap between Uncertainty Quantification and Optimisation and between Probability Theory and Imprecise Probability Theory for Uncertainty Quantification to efficiently solve high-dimensional, expensive and complex engineering problems.

9.3. International Initiatives

9.3.1. Inria Associate Teams Not Involved in an Inria International Labs

9.3.1.1. COMMUNES
Title: Computational Methods for Uncertainties in Fluids and Energy Systems
International Partner (Institution - Laboratory - Researcher):
CWI (Netherlands) - Scientific Computing Group - Daan Crommelin

Start year: 2017
This project aims to develop numerical methods capable to take into account efficiently unsteady experimental data, synthetic data coming from numerical simulation and the global amount of uncertainty associated to measurements, and physical-model parameters. We aim to propose novel algorithms combining data-inferred stochastic modeling, uncertainty propagation through computer codes and data assimilation techniques. The applications of interest are both related to the exploitation of renewable energy sources: wind farms and solar Organic Rankine Cycles (ORCs).

9.3.1.2. HAMster

Title: High order Adaptive moving MeSh finiTE elements in immReSed computational mechanics

International Partner (Institution - Laboratory - Researcher):
Duke (United States) - Civil & Environmental Engineering and Mechanical Engineering & Material Science - Guglielmo Scovazzi

Start year: 2017
See also: https://team.inria.fr/athamster/

This project focuses on adaptive unstructured mesh finite element-type methods for fluid flows with moving fronts. These fronts may be interfaces between different fluids, or fluid/solid, and modelling or physical fronts (e.g. shock waves) present in the flow. The two teams involved in the project have developed over the years complementary strategies, one focusing more on an Eulerian description aiming at capturing fronts on adaptive unstructured grids, the other working more on Lagrangian approaches aiming at following exactly some of these features. Unfortunately, classical Lagrangian methods are at a disadvantage in the presence of complex deformation patterns, especially for fronts undergoing large deformations, since the onset of vorticity quickly leads to mesh rotation and eventually tangling. On the other end, capturing approaches, as well as Immersed Boundary/Embedded (IB/EB) methods, while providing enormous flexibility when considering complex cases, require a careful use of mesh adaptivity to guarantee an accurate capturing of interface physics. The objective of this team is to study advanced hybrid methods combining high order, adaptive, monotone capturing techniques developed in an Eulerian or ALE setting, with fitting techniques and fully Lagrangian approaches.

9.3.2. Inria International Partners

9.3.2.1. Informal International Partners

University of Zurich : R. Abgrall. Collaboration on penalisation on unstructured grids and high order adaptive methods for CFD and uncertainty quantification.

Politecnico di Milano, Aerospace Department (Italy) : Pr. A. Guardone. Collaboration on ALE for complex flows (compressible flows with complex equations of state, free surface flows with moving shorelines).

von Karman Institute for Fluid Dynamics (Belgium). With Pr. T. Magin we work on Uncertainty Quantification problems for the identification of inflow condition of hypersonic nozzle flows. With Pr. H. Deconinck we work on the design of high order methods, including goal oriented mesh adaptation strategies

NASA Langley: Dr. Alireza Mazaheri. Collaboration on high order schemes for PDEs with second and third order derivatives, with particular emphasis on high order approximations of solution derivatives.

Technical University of Crete, School of Production Engineering & Management : Pr. A.I. Delis. Collaboration on high order schemes for depth averaged free surface flow models, including robust code to code validation.
9.4. International Research Visitors

9.4.1. Visits of International Scientists

- From 14/07/17 to 23/07/17 and from 18/12/2017 to 13/01/2018 Guglielmo SCOV AZZI, professor at Duke University, US has visited Mario Ricchiuto to work on...
- From 25/07/2017 to 28/07/2017, Anne EGGELS (PhD / CWI) has visited P.M. Congedo and F. Sanson for working around clustering in UQ methods.
- From 02/2017 to 07/2017, Luca Cirrottola (PhD/ Politecnico di Milano) has visited Cecile Dobrzynski to work on..
- From 2/10/17 to 20/10/2017, Loic GIRALDI , post doc at Ecole Centrale de Nantes has visited P.M. Congedo for working on UQ methods.
- From 13/11/17 to 17/11/2017 Ting SONG (PhD / Duke University) has visited Mario Ricchiuto to work on..
- From 15/12/17 to 07/01/18 Leo NOUVEAU, post doc at Duke University, has visited Héloïse Beaugendre and Mario Ricchiuto to work on..
- From 19/03/17 to 25/03/17, Hossein GORJI, post-doc at the RWTH Aachen University (Germany), has visited Luc Mieussens to work on the modelling of collisions in gases by Fokker-Planck models.
- From 06/09/17 to 13/09/17, Kazuo AOKI, professor at the National Cheng Kung University (Taiwan), has visited Luc Mieussens to work on kinetic modelling of rarefied gases.

9.4.1.1. Internships

- From June 2017 to Sep 2017 Alexandre Bourriaud (Inria, M. Sc. Student)
- From Apr 2017 to Aug 2017 Khawla Msheik (Inria, M. Sc. Student)
- From Jun 2017 to Aug 2017 Loic Hale (Inria, M. Sc. Student)
- From Jun 2017 to Aug 2017 Lola Bouet (Inria, M. Sc. Student)
- From Apr 2017 to Sep 2017 Remi Chassagne (Inria, M. Sc. Student)
- From Mar 2017 to Aug 2017 Saad Abouelfateh (Inria, M. Sc. Student)
- From Jun 2017 to Aug 2017 Stephane Capitaine–Vaillant (Inria, M. Sc. Student)
- From Mar 2017 to Aug 2017 Yamina Hamidi (Inria, M. Sc. Student)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- M. Colin: Modélisation et Analyse des phénomènes dispersifs, conférence en l’honneur de Jean-Claude Saut, ’ENSEIRB MATMECA, 21-27 November 2107, Bordeaux (https://jc70.sciencesconf.org)

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

Mathieu Colin is a member of the scientific committee of The Tenth IMACS International Conference and of the JEF day’s.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

• Mathieu Colin is a member of the board of the journal Applications and Applied Mathematics: An International Journal (AAM)
• P.M. Congedo is Editor of Mathematics and Computers in Simulation, MATCOM (Elsevier)
• Mario Ricchiuto is member of the editorial board of *Computers & Fluids* (Elsevier), and of GEM - International Journal on Geomathematics (Springer)
• A special issue of the European Journal of Mechanics / B Fluids will be dedicated to the 2 editions of the international workshop B’Waves on wave breaking, held in 2014 in Bordeaux (M. Colin and M. Ricchiuto as co-organizers), and in 2016 in Bergen (M. Ricchiuto as co-organizer). M. Colin and M. Ricchiuto will be guest editors of this issue

10.1.3.2. Reviewer - Reviewing Activities


10.1.4. Invited Talks

• Luc Mieussens has been invited to give a talk [35] in the SIAM Conference on Analysis of Partial Differential Equations, Dec 2017, Baltimore, United States.
• M. Ricchiuto has been plenary speaker at the conferences NUMHYP17 in Switzerland (http://www.math.uzh.ch/nmhyp17/index.php?id=speakers), and at the conference Numerical Methods for Shallow Water Equations and Related Models, held in Shenzhen in December 2017 (http://math.sustc.edu.cn/event/10593.html?lang=en).
• P.M. Congedo has been plenary speaker at the conference SimHydro, in June 2017, Nice.

10.1.5. Research Administration

Luc Mieussens is the new director of the "Mesocentre de Calcul Intensif en Aquitaine", started in September, and he has been scientific Advisor for the French Atomic Energy Agency (CEA) for the third year.
10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Doctorat: P.M. Congedo, Introduction to Uncertainty Quantification, 26h, Doctorate School of Politecnico di Milano, Italie.

Master : Héloïse Beaugendre, Calcul Haute Performance (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, France

Master : Héloïse Beaugendre, Responsable de filière de 3ème année, 15h, M2, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Calcul parallèle (MPI), 39h, M2, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Encadrement de projets de la filière Calcul Haute Performance, 10h, M2, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Encadrement de projets sur la modélisation de la pyrolyse, 20h, M1, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Projet fin d’études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin : Integration, M1, 54h, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin : Fortran 90, M1, 44h, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin : PDE, M1, 28h, University of Bordeaux, FRANCE

Master : Mathieu Colin : Analysis, L1, 47h, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin : projet professionnel et internship responsibility : 15 h, ENSEIRB-MATMÉCA, FRANCE

Master : Cécile Dobrzynski, Encadrement de projets TER, 20h, ENSEIRB-MATMÉCA, FRANCE

10.2.2. Supervision

PhD : Arpaia Luca, Continuous mesh deformation and coupling with uncertainty quantification for coastal inundation problems, defended in September 2017.


PhD in progress : Bosi, Umberto, ALE spectral element Boussinesq modelling of wave energy converters, started in November 2015.

PhD in progress : Cortesi Andrea, Predictive numerical simulation for rebuilding freestream conditions in atmospheric entry flows, started in October 2014.

PhD in progress: Lin Xi, Asymptotic modelling of incompressible reactive flows in self-healing composites, started in October 2014.

PhD in progress: Aurore Fallourd, Modeling and Simulation of inflight de-icing systems, Started in October 2016.


PhD in progress: Francois Sanson, Uncertainty propagation in a system of codes, started in February 2016.

PhD in progress: Nassim Razaaly, Robust optimization of ORC systems, started in February 2016.

PhD in progress: Mickael Rivier, Optimization under uncertainties of complex systems, started in May 2017.
10.2.3. Juries

- Luc Mieussens has been referee and member of a jury for the PhD of M. Abdelmalik, defended in TU Eindhoven (Nederlands) in May 2017;
- Héloïse Beagendre has been referee and member of a jury for the PhD of E. Itam (Montpellier University in November 2017), and referee and member of a jury for the PhD of C. Bayeux (ONERA Toulouse, in December 2017);
- Mathieu Colin has been referee and member of a jury for the PhD of Tianxiang Gou, defended in Université de Franche-Comté in October 2017;
- Mario Ricchiuto has been referee and member of the jury of the HDR of J. Harris (U. Paris-Est, November 2017), member of the PhD jury of M. Legal (Paris-Est, February 2017), and president of the juries of J. Deborde (U. de Bordeaux, June 2017), and S. Pelouchon (U. de Bordeaux, November 2017);

11. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journal


Invited Conferences


International Conferences with Proceedings


[22] P. M. CONGEDO, N. RAZAALY, G. IACCARINO. A Gradient Based Local Multivariate Interpolation Regression Surrogate Model for scattered data sets, in "UNCECOMP 2017 - 2nd International Conference on Uncertainty Quantification in Computational Sciences and Engineering", Rhodes, Greece, June 2017, https://hal.inria.fr/hal-01671010.


Conferences without Proceedings


Scientific Books (or Scientific Book chapters)


**Research Reports**


[50] N. RAZAALY, P. M. CONGEDO. *Novel algorithm using Active Metamodel Learning and Importance Sampling: application to multiple failure regions of low probability*, Inria Bordeaux, équipe CARDAMOM, June 2017, n° RR-9079, 30, https://hal.inria.fr/hal-01550770.


**Other Publications**

References in notes


[66] S. BELLEC, M. COLIN, M. RICCHIUTO. *Discrete asymptotic equations for long wave propagation*, Inria Bordeaux Sud-Ouest, November 2015, n° RR-8806. [https://hal.inria.fr/hal-01224157](https://hal.inria.fr/hal-01224157).


A flexible genuinely nonlinear approach for wave propagation, breaking and runup, Inria Bordeaux Sud-Ouest ; Inria, June 2015, n° RR-8746, https://hal.inria.fr/hal-01166295.


Numerical study of wave conditions for the old Venetian harbour of Chania in Crete, Greece, in "36th International Association for Hydro-Environment Engineering and Research (IAHR) World Conference", The Hague, Netherlands, June 2015.


Project-Team CARMEN

Modélisation et calculs pour l’électrophysiologie cardiaque

IN PARTNERSHIP WITH:
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences
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Project-Team CARMEN

Creation of the Team: 2011 October 01, updated into Project-Team: 2016 June 01

Keywords:

**Computer Science and Digital Science:**
- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.4. - Multiscale modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.2.6. - Optimization
- A6.2.7. - High performance computing
- A6.2.8. - Computational geometry and meshes
- A6.3. - Computation-data interaction
- A6.3.1. - Inverse problems
- A6.3.2. - Data assimilation
- A6.3.3. - Data processing
- A6.3.4. - Model reduction
- A6.3.5. - Uncertainty Quantification

**Other Research Topics and Application Domains:**
- B1.1.3. - Cellular biology
- B1.1.9. - Bioinformatics
- B1.1.11. - Systems biology
- B2.2.1. - Cardiovascular and respiratory diseases
- B2.4.1. - Pharmaco kinetics and dynamics
- B2.6.2. - Cardiac imaging

1. Personnel

**Research Scientists**
- Jacques Henry [Inria, Emeritus, HDR]
- Michael Leguèbe [Inria, Researcher, from Oct 2017]
- Mark Potse [Inria, Advanced Research Position]
- Nejib Zemzemi [Inria, Researcher]

**Faculty Members**
- Yves Couderie [Team leader, Univ de Bordeaux, Professor, HDR]
- Mostafa Bendahmane [Univ de Bordeaux, Associate Professor]
- Lisl Weynans [Univ de Bordeaux, Associate Professor, from Jun 2017]

**External Collaborators**
- Jason Bayer [Univ de Bordeaux]
- Gwladys Ravon [Univ de Bordeaux]
- Edward Vigmond [Univ de Bordeaux]

**Technical Staff**
- Andjela Davidovic [Inria, granted by ANR /13-HR-CEM project]
- Mehdi Juhoor [Inria, granted by PRES Univ de Bordeaux]
- Pauline Migerditichan [Inria]
2. Overall Objectives

2.1. Overall Objectives

The Carmen team develops and uses models and numerical methods to simulate the electrophysiology of the heart from the molecular to the whole-organ scale, and its relation to measurable signals inside the heart and on the body surface. It aims at

- improving understanding of normal and pathological cardiac electrophysiology,
- improving the efficiency and accuracy of numerical models, and
- exploitation of all available electrical signals for diagnosis, in particular for prediction of life-threatening cardiac arrhythmias.

The numerical models used and developed by the team incorporate the gating dynamics of the ion channels in the cardiac cell membranes and the heterogeneities and coupling processes on the cellular scale into macroscopic reaction-diffusion models. At the same time we use reduced models to solve the inverse problems related to non-invasive electrical imaging of the heart.

The fields involved in our research are: ordinary and partial differential equations (PDE), inverse problems, numerical analysis, high-performance computing, image segmentation, and mesh construction.

A main goal of the team is to contribute to the work packages defined in the IHU LIRYC (http://ihu-liryc.fr), an institute founded in 2011 that focuses on cardiac arrhythmia.

We cooperate with physiologists and cardiologists on several projects. The team is building new models and powerful simulation tools that will help to understand the mechanisms behind cardiac arrhythmias and to establish personalized and optimized treatments. A particular challenge consists in making the simulations reliable and accessible to the medical community.
3. Research Program

3.1. Complex models for the propagation of cardiac action potentials

The contraction of the heart is coordinated by a complex electrical activation process which relies on about a million ion channels, pumps, and exchangers of various kinds in the membrane of each cardiac cell. Their interaction results in a periodic change in transmembrane potential called an action potential. Action potentials in the cardiac muscle propagate rapidly from cell to cell, synchronizing the contraction of the entire muscle to achieve an efficient pump function. The spatio-temporal pattern of this propagation is related both to the function of the cellular membrane and to the structural organization of the cells into tissues. Cardiac arrhythmias originate from malfunctions in this process. The field of cardiac electrophysiology studies the multiscale organization of the cardiac activation process from the subcellular scale up to the scale of the body. It relates the molecular processes in the cell membranes to the propagation process and to measurable signals in the heart and to the electrocardiogram, an electrical signal on the torso surface.

Several improvements of current models of the propagation of the action potential are being developed in the Carmen team, based on previous work [49] and on the data available at IHU LIRYC:

- Enrichment of the current monodomain and bidomain models [49], [59] by accounting for structural heterogeneities of the tissue at an intermediate scale. Here we focus on multiscale analysis techniques applied to the various high-resolution structural data available at the LIRYC.
- Coupling of the tissues from the different cardiac compartments and conduction systems. Here, we develop models that couple 1D, 2D and 3D phenomena described by reaction-diffusion PDEs.

These models are essential to improve our in-depth understanding of cardiac electrical dysfunction. To this aim, we use high-performance computing techniques in order to numerically explore the complexity of these models.

We use these model codes for applied studies in two important areas of cardiac electrophysiology: atrial fibrillation [51] and sudden-cardiac-death (SCD) syndromes [7], [6] [54]. This work is performed in collaboration with several physiologists and clinicians both at IHU Liryc and abroad.

3.2. Simplified models and inverse problems

The medical and clinical exploration of the cardiac electric signals is based on accurate reconstruction of the patterns of propagation of the action potential. The correct detection of these complex patterns by non-invasive electrical imaging techniques has to be developed. This problem involves solving inverse problems that cannot be addressed with the more complex models. We want both to develop simple and fast models of the propagation of cardiac action potentials and improve the solutions to the inverse problems found in cardiac electrical imaging techniques.

The cardiac inverse problem consists in finding the cardiac activation maps or, more generally, the whole cardiac electrical activity, from high-density body surface electrocardiograms. It is a new and a powerful diagnosis technique, which success would be considered as a breakthrough. Although widely studied recently, it remains a challenge for the scientific community. In many cases the quality of reconstructed electrical potential is not adequate. The methods used consist in solving the Laplace equation on the volume delimited by the body surface and the epicardial surface. Our aim is to

- study in depth the dependance of this inverse problem on inhomogeneities in the torso, conductivity values, the geometry, electrode positions, etc., and
- improve the solution to the inverse problem by using new regularization strategies, factorization of boundary value problems, and the theory of optimal control, both in the quasistatic and in the dynamic contexts.
Of course we will use our models as a basis to regularize these inverse problems. We will consider the following strategies:

- using complete propagation models in the inverse problem, like the bidomain equations, for instance in order to localize electrical sources;
- constructing families of reduced-order models using e.g. statistical learning techniques, which would accurately represent some families of well-identified pathologies; and
- constructing simple models of the propagation of the activation front, based on eikonal or level-set equations, but which would incorporate the representation of complex activation patterns.

Additionally, we will need to develop numerical techniques dedicated to our simplified eikonal/level-set equations.

### 3.3. Numerical techniques

We want the numerical simulations of the previous direct or inverse models to be efficient and reliable with respect to the needs of the medical community. They should qualify and guarantee the accuracy and robustness of the numerical techniques and the efficiency of the resolution algorithms.

Based on previous work on solving the monodomain and bidomain equations [4], [5], [8], [1], we will focus on

- High-order numerical techniques with respect to the variables with physiological meaning, like velocity, AP duration and restitution properties.
- Efficient, dedicated preconditioning techniques coupled with parallel computing.

Existing simulation tools used in our team rely, among others, on mixtures of explicit and implicit integration methods for ODEs, hybrid MPI-OpenMP parallelization, algebraic multigrid preconditioning, and a BiCGStab algorithm with adaptations to retain numerical accuracy while handling large underdetermined systems.

### 3.4. Cardiac Electrophysiology at the Microscopic Scale

Numerical models of whole-heart physiology are based on the approximation of a perfect muscle using homogenisation methods. However, due to aging and cardiomyopathies, the cellular structure of the tissue changes. These modifications can give rise to life-threatening arrhythmias. For our research on this subject and with cardiologists of the IHU LIRYC Bordeaux, we aim to design and implement models that describe the strong heterogeneity of the tissue at the cellular level and to numerically explore the mechanisms of these diseases.

The literature on this type of model is still very limited [63]. Existing models are two-dimensional [55] or limited to idealized geometries, and use a linear (purely resistive) behaviour of the gap-junction channels that connect the cells. We propose a three-dimensional approach using realistic cellular geometry (figure 1), nonlinear gap-junction behaviour, and a numerical approach that can scale to hundreds of cells while maintaining a sub-micrometer spatial resolution (10 to 100 times smaller than the size of a cardiomyocyte) [28] [48], [47].

### 4. Application Domains

#### 4.1. Scientific context: the LIRYC

The University Hospital of Bordeaux (CHU de Bordeaux) is equipped with a specialized cardiology hospital, the Hôpital Cardiologique du Haut-Lévêque, where the group of Professor Michel Haïssaguerre has established itself as a global leader in the field of cardiac electrophysiology [53], [52], [45]. Their discoveries in the area of atrial fibrillation and sudden cardiac death syndromes are widely acclaimed, and the group is a national and international referral center for treatment of cardiac arrhythmia. Thus the group also sees large numbers of patients with rare cardiac diseases.
Figure 1. **A:** The cardiac muscle consists of a branching network of elongated muscle cells, interspersed with other structures. Sheets of connective tissue (blue) can grow between the muscle cells and become pathogenic. **B:** Current models can only represent such alterations in a coarse way by replacing model elements with different types; each cube in this illustration would represent hundreds of cells. **C:** This hand-crafted example illustrates the type of geometric model we are experimenting with. Each cell is here represented by hundreds of elements.

In 2011 the group has won the competition for a 40 million euro *Investissements d’Avenir* grant for the establishment of IHU Liry, an institute that combines clinical, experimental, and numerical research in the area of cardiac arrhythmia (http://ihu-liryc.fr). The institute works in all areas of modern cardiac electrophysiology: atrial arrhythmias, sudden death due to ventricular fibrillation, heart failure related to ventricular dyssynchrony, and metabolic disorders. It is recognized as one of the most important centers worldwide in this area.

The Carmen team was founded to partner with IHU Liry. We bring applied mathematics and scientific computing closer to experimental and clinical cardiac electrophysiology. In collaboration with experimental and clinical researchers at Liry we work to enhance fundamental knowledge of the normal and abnormal cardiac electrical activity and of the patterns of the electrocardiogram, and we develop new simulation tools for training, biological, and clinical applications.

### 4.2. Basic experimental electrophysiology

Our modeling is carried out in coordination with the experimental teams from IHU Liry. It help to write new concepts concerning the multiscale organisation of the cardiac action potentials that will serve our understanding in many electrical pathologies. For example, we model the structural heterogeneities at the cellular scale [28], and at an intermediate scale between the cellular and tissue scales.

At the atrial level, we apply our models to understand the mechanisms of complex arrhythmias and the relation with the heterogeneities at the insertion of the pulmonary veins. We will model the heterogeneities specific to the atria, like fibrosis or fatty infiltration [51]. These heterogeneities ar thought to play a major role in the development of atrial fibrillation.

At the ventricular level, we focus on (1) modeling the complex coupling between the Purkinje network and the ventricles and (2) modeling the heterogeneities related to the complex organization and disorganization of the myocytes and fibroblasts. Point (1) is supposed to play a major role in sudden cardiac death and point (2) is important in the study of infarct scars for instance.

### 4.3. Clinical electrophysiology

Treatment of cardiac arrhythmia is possible by pharmacological means, by implantation of pacemakers and defibrillators, and by curative ablation of diseased tissue by local heating or freezing. In particular the ablative therapies create challenges that can be addressed by numerical means. Cardiologists would like to know, preferably by noninvasive means, where an arrhythmia originates and by what mechanism it is sustained.
We address this issue in the first place using inverse models, which attempt to estimate the cardiac activity from a (high-density) electrocardiogram. A new project aims at performing this estimation on-site in the catheterization laboratory and presenting the results, together with the cardiac anatomy, on the screen that the cardiologist uses to monitor the catheter positions [25].

An important prerequisite for this kind of interventions and for inverse modeling is the creation of anatomical models from imaging data. The Carmen team contributes to better and more efficient segmentation and meshing through the IDAM project.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

Michał Kania received a Gary and Bill Sanders poster award for his contribution “Prediction of the Exit Site of Ventricular Tachycardia Based on Different ECG Lead Systems” to the Computing in Cardiology meeting in Rennes, September 2017.

5.1.2. Inria domain evaluation

In October the Carmen team participated in the evaluation of the Inria domain Life sciences, theme Modelling and Control for Life Sciences, during a 3-day seminar in Paris. The report was very positive about our work in general. The jury, composed of high-profile international scientists, noted especially the development of a bilayer model of the atria [56], [50] [15], the modified monodomain model which can reproduce much of the much more expensive bidomain model [49], and our contributions to electrocardiographic imaging [24], [17], [23], [27].

Best Papers Awards:

6. New Software and Platforms

6.1. CEPS

Cardiac ElectroPhysiology Simulation
Keywords: 3D - Cardiac - Mesh - Health - Simulation - Cardiac Electrophysiology
Scientific Description: As compared to other existing softwares, CEPS aims at providing a more general framework of integration for new methods or models and a better efficiency in parallel. CEPS is designed to run on massively parallel architectures, and to make use of state-of-the-art and well known computing libraries to achieve realistic and complex heart simulations. CEPS also includes software engineering and and validation tools.
Functional Description: CEPS is a numerical simulation tool focused on the modeling of cardiac electrophysiology. The goal of CEPS is to easily allow the development of new numerical methods and new physical models.

- Participants: Mehdi Juhoor and Nejib Zemzemi
- Partners: Université de Bordeaux - CNRS - INP Bordeaux - IHU - LIRYC
- Contact: Yves Coudière
- URL: https://gforge.inria.fr/projects/ceps/
6.2. Platforms

6.2.1. CEMPACK

CEMPACK is a new collection of software that was previously archived in different places. It includes the high-performance simulation code Propag and a suite of software for the creation of geometric models, preparing inputs for Propag, and analysing its outputs. In the course of 2017 the code was collected in an archive on Inria’s GitLab platform, and a public website was created where documentation will be placed (http://cempack.gforge.inria.fr).

The main components of CEMPACK are the following.
- Propag-5.1 Applied modeling studies performed by the Carmen team, especially M. Potse and M. Kania, in collaboration with IHU Liryc and foreign partners [17] [7] [61], [51] [43] rely to a great extent on high-performance computations on the national supercomputers Curie, Occigen, and Turing. The Propag-5 code is optimized for these systems. It is the result of a decades-long development first at the *Université de Montréal* in Canada, then at Maastricht University in the Netherlands, and finally at the Institute of Computational Science of the *Università della Svizzera italiana* in Lugano, Switzerland. Since 2016 most of the development on Propag has been done by M. Potse at the Carmen team. The code scales excellently to large core counts and, as it is controlled completely with command-line flags and configuration files, it can be used by non-programmers. It also features
  - a plugin system for membrane models,
  - a completely parallel workflow, including the initial anatomy input and mesh partitioning, which allows it to work with meshes of more than $10^9$ nodes,
  - a flexible output scheme allowing hundreds of different state variables and transient variables to be output to file, when desired, using any spatial and temporal subsampling,
  - a configurable, LUSTRE-aware parallel output system in which groups of processes write HDF5/netCDF files, and
  - CWEB documentation of the entire code base.

The code has been stable and reliable for several years, and only minor changes are being made currently. It can be considered the workhorse for our HPC work until CEPS takes over.

- Gepetto The Gepetto suite, named after a famous model maker, transforms a surface mesh of the heart into a set of (semi-)structured meshes for use by the Propag software or others. It creates the different fiber orientations in the model, including the transmurally rotating ventricular fibers and the various bundle structures in the atria (figure 2), and creates layers with possibly different electrophysiological properties across the wall. A practically important function is that it automatically builds the matching heart and torso meshes that Propag uses to simulate potentials in the torso (at a resolution of $1$ mm) after projecting simulation results from the heart model (at $0.1$ to $0.2$ mm) on the coarser torso mesh [60]. Like Propag, the Gepetto software results from a long-term development that started in Montreal, Canada, around 2002. The code for atrial fiber structure was developed by our team.

- Blender plugins Blender (https://www.blender.org) is a free software package for the production of 3-D models, renderings, and animations, comparable to commercial software such as Cinema4D. CEMPACK includes a set of plugins for Blender that facilitate the production of anatomical models and the visualization of data. It uses the MMG remeshing library, which is developed by the CARDAMOM team at Inria Bordeaux.

6.2.2. MUSIC

MUSIC is a multimodal platform for cardiac imaging developed by the imaging team at IHU LIRYC in collaboration with the Inria team Asclepios (https://bil.inria.fr/fr/software/view/1885/tab). It is based on the medInria software also developed by the Asclepios team. MUSIC is a cross-platform software for segmentation of medical imaging data, meshing, and ultimately also visualization of functional imaging data and model results.
7. New Results

7.1. A parameter optimization method to solve the ECG inverse problem

Existing electrocardiographic inverse models express their results either in terms of potentials on the heart surface or in terms of activation times in the heart. G. Ravon developed a new method which gives a potentially more useful answer in terms of three parameters of the underlying action potentials in the heart [27]. Since there are more parameters, care had to be taken to avoid overfitting. Tests on in-silico and ex-vivo data showed good results: the method gave better activation maps than the method of fundamental solutions to which it was compared, and fitted the repolarization phase of the ECG accurately. Figure shows an example of an inversely estimated repolarization map.

7.2. Optimal control to Bidomain-Bath model

This project is concerned with the study of the convergence analysis for an optimal control of a bidomain-bath model. The bidomain-bath model equations describe the cardiac bioelectric activity at the tissue bath volumes where the control acts at the boundary of the tissue domain. In recent work [13] [44], we established the well-posedeness of the direct bidomain-bath model by a discrete Galerkin approach. The convergence proof is based on deriving a series of a priori estimates and using a general $L^2$-compactness criterion. Moreover, the well-posedeness of the adjoint problem and the first order necessary optimality conditions are shown. Comparing to the direct problem, the convergence proof of the adjoint problem is based on using a general $L^1$-compactness criterion. The numerical tests are demonstrated which achieve the successful cardiac defibrillation by utilizing less total current. Finally, the robustness of the Newton optimization algorithm is presented for different finer mesh geometries.
7.3. Bidomain Calcium Dynamics in Cardiac Cell

In our project [35], we are interested in modeling the interaction of Calcium dynamics in a bidomain medium including Sarcolemma and Sarcoplasmic reticulum. The governing equations consist of a nonlinear reaction-diffusion system representing the various calcium fluxes and their buffers in the two medias. A priori stability bounds and the solvability of the system is analyzed using a fixed-point approach. We introduce a finite element method to numerically solve our model equations. Moreover, we establish existence of discrete solutions and show convergence to a weak solution of the original problem. Finally, we report several 2D and 3D numerical experiments illustrating the behavior of the proposed scheme.

7.4. Cardiac electromechanics with physiological ionic model

This project [37] is concerned with the mathematical analysis of a coupled elliptic-parabolic system modeling the interaction between the propagation of electric potential coupled with general physiological ionic models and subsequent deformation of the cardiac tissue. A prototype system belonging to this class is provided by the electromechanical bidomain model, which is frequently used to study and simulate electrophysiological waves in cardiac tissue. The coupling between muscle contraction, biochemical reactions and electric activity is introduced with a so-called active strain decomposition framework, where the material gradient of deformation is split into an active (electrophysiology-dependent) part and an elastic (passive) one. We prove existence of weak solutions to the underlying coupled electromechanical bidomain model under the assumption of linearized elastic behavior of the updated nonlinear diffusivities. The proof of the existence result is proved by means of a non-degenerate approximation system, the Faedo-Galerkin method, and the compactness method.

7.5. Electrocardiographic lead fields

Currently a monodomain reaction-diffusion model is a well-established method to simulate the electrical activity of the heart [58], [59], even more so because it can be adapted to approximate a bidomain model very closely [46], [49]. Computing the electrocardiogram (ECG) from the results of such models is harder because it requires large linear systems to be solved, and does not scale well to large numbers of processors. A possible solution is to use so-called lead fields, the electrocardiographic term for a linear combination of Green’s functions that express the ECG potential as an integral over a field of electric current dipoles. M. Poëte has implemented and tested methods to compute and use lead fields for ECG simulation with the Propag code. It turned out that this classical method is practical and sufficiently accurate, and gives a huge scaling advantage on modern highly parallel computers. This result is of practical importance for our applied work, and a journal manuscript on this topic will be submitted in January 2018.
7.6. Rapid localization of arrhythmia

Our pilot studies using model data [25] have shown promising results for a proposed simple and rapid localization method to be used in the catheterization laboratory. We have found that even with only a few ECG electrodes accuracies in the order of millimeters can be achieved for the position of an arrhythmia origin with respect to a catheter position. A journal manuscript on this topic is expected to be complete in February 2018.

7.7. Bilayer model

The rigorous proof that mathematically found the bilayer model from S. Labarthe PhD thesis [56] was actually published in SIAM Journal of Applied Math [15]. Based on sophisticated energy estimates, it proves that the bilayer model is the rigorous limit of the underlying three-dimensional model.

7.8. multi-electrode array measurement

In the context of the CardioXComp project, in collaboration with the REO team and the company Notocord, we proposed a strategy to analyze the signals acquired by multi-electrode array (MEA) on cultures of hiPSC-CMs cells with drug compounds, and to automatically deduce the channels affected by the drug. First, in [10], we study how MEA measurement can be modeled in such a way that the produced in-silico signals are comparable to real ones. The main problems concern the heterogeneities of cell cultures. Then, in [20] a method based on parameter identification, by comparing the in-silico and real signals, was used on signals acquired with commercial systems on cell culture with various drugs. The IC-50 and dose-response of several drugs could be assessed. This kind of techniques could contribute to promote the technology based on MEA and hiPSC-CMs.

7.9. High-order integration methods for ion channel models

On November 15, 2017, C. Douanla Lontsi defended his PhD thesis [9] on the numerical analysis of time-stepping methods for the cardiac monodomain equations. A huge amount of work was carried out in the thesis. The thesis builds on the seminal Rush-Larsen technique [62], [57], and the recent novel computational interest in exponential integrator methods. Two new exponential methods of arbitrarily high order are proposed (EABk and RLk). Most notably, Rush-Larsen techniques of order \( k = 2, 3, 4 \) were entirely explicated. The theory was adapted to analyse these methods and convergence proofs were derived. The complete Dahlquist stability region of these methods was documented. Finally, the methods were integrated into an IMEX strategy to solve the monodomain equation in 1D to 3D problems, with two ionic models (BR and TNNP). The results essentially show that order at least 3 is required to lead to reasonably accurate simulations. Three journal papers were submitted in 2017, [39], [41], [40].

7.10. High-order finite-volume discretizations

Y. Coudière and R. Turpault proposed new simple and efficient high-order finite volume discretizations to be applied to the monodomain equation. They showed how the method can be easily implemented up to the order 6, with very good results, also for simulation of complex propagation patterns. The results were published in [16].

7.11. Identification of multiple space dependent ionic parameters in cardiac electrophysiology modelling

In this paper, we consider the inverse problem of space dependent multiple ionic parameters identification in cardiac electrophysiology modelling from a set of observations. We use the monodomain system known as a state-of-the-art model in cardiac electrophysiology and we consider a general Hodgkin-Huxley formalism to describe the ionic exchanges at the microscopic level. This formalism covers many physiological transmembrane potential models including those in cardiac electrophysiology. Our main result is the proof of the uniqueness and a Lipschitz stability estimate of ion channels conductance parameters based on some observations on an arbitrary subdomain.
8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. CALM

The project “Cardiac Arrhythmia Localization Methods” has been granted by the Région Nouvelle-Aquitaine, with matching from funds held by our clinical collaborators Dr. Hubert Cochet and Dr. Pierre Jais, and from Inria. The purpose of this project is to develop a tool that can predict the exit site of an arrhythmia with moderate accuracy (1 cm) in an absolute sense, with respect to the anatomy of the heart in situ, and with a resolution of about 2 mm in a relative sense, with respect to a nearby pacing site. This tool must fulfill the following criteria:

- it uses only data that are already recorded in the cathlab by other systems: ECG data and electroanatomical mapping data;
- it must work in nearly real-time; catheter displacement advice must be available within 5 seconds after a paced beat;
- it must work automatically, requiring the operator only to indicate which ECG data correspond to the target arrhythmia; and
- it must be safe and easy to operate.

We will in the first place test a number of proposed methods using synthetic data, produced with our realistic models of cardiac electrophysiology and accurate geometric models of different patients. This in-silico testing phase will answer a number of important practical questions. Subsequently we will use offline clinical data, and within 2 years we aim to build a clinical prototype that can be tested (without interfering in the procedure) in the cathlab. In order to work real-time we will initially use very simple methods. However, the clinical prototype and the collectoin of synthetic data that we created will later serve also as a platform to test also more sophisticated inverse methods.

8.1.2. EXACARD

We started a collaboration with the STORM team at Inria Bordeaux Sud-Ouest to work on further scaling of the Propag code, to push the limit from about $10^4$ to $10^6$ parallel processors. A pre-proposal has been submitted to the ANR, and we are doing preparatory work.

8.2. National Initiatives

8.2.1. ANR HR-CEM

The project “High Resolution Cardiac Electrophysiology Models: HR-CEM” within the ANR call *Modèles Numériques* started in November 2013 and lasted until November 2017.

This international project involved three partners: Inria (coordinator), IHU LIRYC, and UMI-CRM in Montréal (Canada). The project has external collaborators in Univ. Bordeaux and Univ. Pau.

Based on these collaborations and new developments in structural and functional imaging of the heart available at LIRYC, we plan to reconsider the concepts behind the models in order to improve the accuracy and efficiency of simulations. Cardiac simulation software and high-resolution numerical models will be derived from experimental data from animal models. Validation will be performed by comparing of simulation output with experimentally recorded functional data. The validated numerical models will be made available to the community of researchers who take advantage of in-silico cardiac simulation and, hopefully, become references. In particular we shall provide the first exhaustive model of an animal heart including the four chambers coupled through the special conduction network, with highly detailed microstructure of both the atria and the ventricles. Such a model embedded in high-performance computational software will provide stronger medical foundations for in-silico experimentation, and elucidate mechanisms of cardiac arrhythmias.
8.2.2. ANR MITOCARD

The MITOCARD project (Electrophysiology of Cardiac Mitochondria), coordinated by S. Arbault (Université de Bordeaux, ISM), was granted by the ANR in July 2017. The objective of MITOCARD is to improve understanding of cardiac physiology by integrating the mitochondrial properties of cell signaling in the comprehensive view of cardiac energetics and rhythm pathologies. It was recently demonstrated that in the heart, in striking contrast with skeletal muscle, a parallel activation by calcium of mitochondria and myofibrils occurs during contraction, which indicates that mitochondria actively participate in Ca2+ signaling in the cardiomyocyte. We hypothesize that the mitochondrial permeability transition pore (mPTP), by rhythmically depolarizing inner mitochondrial membrane, plays a crucial role in mitochondrial Ca2+ regulation and, as a result, of cardiomyocyte Ca2+ homeostasis. Moreover, mitochondrial reactive oxygen species (ROS) may play a key role in the regulation of the mPTP by sensing mitochondrial energetics balance. Consequently, a deeper understanding of mitochondrial electrophysiology is mandatory to decipher their exact role in the heart’s excitation-contraction coupling processes. However, this is currently prevented by the absence of adequate methodological tools (lack of sensitivity or selectivity, time resolution, averaged responses of numerous biological entities). The MITOCARD project will solve that issue by developing analytical tools and biophysical approaches to monitor kinetically and quantitatively the Ca2+ handling by isolated mitochondria in the cardiomyocyte.

MITOCARD is a multi-disciplinary project involving 4 partners of different scientific fields: the CARMEN team as well as

ISM, the largest chemistry laboratory of the Université de Bordeaux, where the necessary measurement methods will be developed;
Liryc, where mitochondria are studied at all levels of integration from the isolated mitochondrion to the intact heart; and
LAAS, the MiCrosystèmes d’Analyse (MICA) group at the Laboratory of Analysis and Architecture of Systems, which develops the biological microsensors for this project.

The project will
- develop chips integrating 4 different electrochemical microsensors to monitor in real-time key mitochondrial signaling parameters: Ca2+, membrane potential, quinone reduction status, O2 consumption, and ROS production;
- develop microwell arrays integrating ring nanoelectrodes to trap single mitochondria within micrometric chambers and measure locally by combined fluorescence microscopy and electrochemical techniques intra- (by fluorescence) and extra-mitochondrial (electrochemistry) metabolites; and
- develop a mathematical model of mitochondrial Ca2+ and ROS handling built on existing knowledge, new hypotheses, and the measured data.

The model may serve both to assess biological assumptions on the role of mitochondria in Ca2+ signaling and to integrate pathological data and provide clues for their global understanding.

8.2.3. GENCI

GENCI (grand équipement national de calcul intensif) is the agency that grants access to all national high-performance resources for scientific purposes in France. GENCI projects have to be renewed yearly. Our project renewal Interaction between tissue structure and ion-channel function in cardiac arrhythmia, submitted in September 2017, has been granted 9 million core-hours on the three major systems Curie, Occigen, and Turing. This compute time is primarily destined for our research into the interaction between ionic and structural heart disease in atrial fibrillation, Brugada syndrome, and early repolarisation syndrome [7] [61].

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

We participated in two H2020 Research and Innovation Action proposals.
8.3.2. Collaborations in European Programs, Except FP7 & H2020

We coordinated a proposal with 5 European partners. The proposal could not be submitted due to administrative problems related to one of the partners, but we will benefit from the existing consortium to submit a new proposal in April 2018.

8.4. International Initiatives

8.4.1. Inria International Labs

8.4.1.1. EPICARD

Title: inversE Problems In CARDiac electrophysiology
International Partner (Institution - Laboratory - Researcher):

ENIT (Tunisia) – Department of Intelligence Science and Technology - Nabil Gmati

Start year: 2015
See also: https://team.inria.fr/carmen/epicard/

Improving the information that we can extract from electrical signals measured on patients with heart diseases is a major priority for the IHU LIRYC in Bordeaux headed by Professor Michel Haïssaguerre. We would like to non-invasively construct the electrical potential on the heart surface only from measurements of the electrical potential on the chest of the patient.

This helps the medical doctor to visualise an image of the electrical potential of the heart of the patient. It is known that have been used in the literature for solving this electrocardiography imaging (ECGI) problem, including those used in commercial medical devices have several limitations. This problem could be mathematically seen as a boundary data completion problem for elliptic equations.

Many works in the literature have been carried out in order to solve this Cauchy problem, but have never been used for solving the ECGI problem. Our goal from the associate team is to develop an experimental platform allowing to test various methods and compare their performance on real life experimental data.

8.4.2. Inria International Partners

8.4.2.1. Informal International Partners

Y. Coudière works with the group of Prof. Y. Bourgault from the Department of Mathematics and Statistics of the University of Ottawa (Canada). Some results on the numerical analysis of time-stepping methods from C. Douanla’s PhD were carried out together, as well as some theoretical results on parameter identification in the PhD of A. Gérard.

M. Potse and O. Bernus (Liryc) work with the group of Prof. A. Panfilov in Ghent, Belgium, on simulation and analysis of complex reentrant arrhythmia.

M. Potse works with the group of Prof. U. Schotten at Maastricht University (The Netherlands) and the Center for Computational Medicine in Cardiology at the Università della Svizzera italiana (Lugano, Switzerland) on simulation studies of atrial fibrillation [51]. The Maastricht group was partially funded by the FP7 project EUTRAF and our simulations were supported by GENCI (section 8.2.3).

M. Potse set up a project and recruited a PhD student to co-direct with Dr. Esther Pueyo of the University of Zaragoza, within the context of the H2020 International Training Network “Personalised In-silico Cardiology” (PIC), coordinated by Dr. Pablo Lamata of King’s College London.

N. Zemzemi works with Cesare Corrado at King’s College London on the development of new eikonal models allowing conduction velocity adaptation [14].

N. Zemzemi collaborated with Jesús Requena-Carrión from the Queen Mary University of London to study the effects of the spatial resolution of electrode systems on the spectrum of cardiac signals in cardiac electrocardiography [12].
N. Zemzemi worked with R. Aboulaich group from Mohamed V university in Morocco on sensitivity of the electrocardiographic problem to multiple independent sources of uncertainty including noise in the measurements and the heterogeneity in the torso [34].

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

Y. Coudière co-organised the Workshop on Mathematical Methods in Cardiac Electrophysiology, November 4–6, 2017, at the University of Ottawa in Canada. Approximately 30 scientists from the US, Canada, and several European countries participated in this workshop.

9.1.2. Scientific Events Selection

9.1.2.1. Member of the Conference Program Committees

Y. Coudière was a program committee member for the Functional Imaging and Modeling of the Heart (FIMH) meeting 2017 in Toronto, Canada.

M. Potse is a track chair for the International Congress of Cardiology 2018 in Chiba, Japan.

9.1.2.2. Reviewer

Y. Coudière and M. Potse reviewed abstracts for the Computing in Cardiology meeting in Rennes, September 2017.

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

M. Potse: associate editor of Frontiers in Cardiac Electrophysiology.

9.1.3.2. Reviewer - Reviewing Activities

L. Weynans: Computers and Fluids, Multiscale Modeling and Simulation


Y. Coudière: Journal of computational and applied mathematics, PLOS ONE, SMAI Journal of Computational Mathematics


9.1.4. Invited Talks


### 9.1.5. Leadership within the Scientific Community

M. Potse is council member of the International Society of Electrocardiology.

### 9.1.6. Research Administration

L. Weynans: member of the “Conseil du département Sciences et Technologies” of Bordeaux University.

Y. Coudière:
- Scientific responsibility of the IMB (CNRS UMR 5251) team “Calcul Scientifique et Modélisation,” \( \sim 60 \) persons.
- Responsible for the scientific communication (*Chargé de mission à l’animation scientifique*) of the IMB.
- N. Zemzemi: Administration of the Inria associated team Epicard.

M. Leguèbe: co-organization of team “Calcul Scientifique et Modélisation” seminar.

### 9.2. Teaching - Supervision - Juries

#### 9.2.1. Teaching

<table>
<thead>
<tr>
<th>Licence</th>
<th>Master</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y. Coudière, Groupe de Travail Applicatif, 33h,L2, Université de Bordeaux, France</td>
<td>Y. Coudière, Méthodes d’éléments finis pour la mécanique des fluides incompressibles, 33h, M2, Université de Bordeaux, France</td>
</tr>
</tbody>
</table>

Licence : Y. Coudière, Projet multidisciplinaire Matmeca, 33h, L2, Université de Bordeaux, France.

Licence : M. Bendahmane, Mathématiques générales, 36h, L1, Université de Bordeaux, France.

Licence : M. Bendahmane, Algèbre Linéaire, 46h, L2, Université de Bordeaux, France.

Licence : M. Bendahmane, Fonctions de plusieurs variables et optimisation, 33h, L2, Université de Bordeaux, France.

Licence : M. Bendahmane, Analyse appliquée, 33h, L1, Université de Bordeaux, France.

Licence : M. Bendahmane, Séries et intégrales multiples, 33h, L1, Université de Bordeaux, France.

Master : M. Bendahmane, Analyse appliquée, 33h, M2, Université de Bordeaux, France.

Licence : L. Weynans, Fortran MMK, 20h, L1, Université de Bordeaux, France.

Licence : L. Weynans, Introduction Analyse Numérique, 24h, L3, Université de Bordeaux, France.

Licence : L. Weynans, Cours Programmation avancée pour le calcul scientifique, 24h, L3, Université de Bordeaux, France.

Licence : L. Weynans, TP Programmation avancée pour le calcul scientifique, 34h, L3, Université de Bordeaux, France.

Licence : L. Weynans, encadrement de projets 1ère année Matmeca, 25h, L1, Université de Bordeaux, France.

Y. Coudière is responsible for the program “Ingénierie mathématique” in the Mathematics Bachelor, and responsible for the program “Modélisation Numérique et Calcul Haute Performance” in the Master program Applied Mathematics and Statistics, at the Université de Bordeaux.
9.2.2. Supervision


PhD in progress: A. Gérard, “Modèles numériques personnalisés de la fibrillation auriculaire,” started 1 September 2015, supervised by Y. Coudière.

PhD in progress: B. Lambert, “Modélisation et simulation numérique de suspensions de particules dans un fluide,” started 1 October 2015, supervised by M. Bergmann and L. Weynans.

PhD : N. Fikal, “Quantification d’incertitudes en électrocardiographie par la méthode éléments finis stochastique,” Université de Mohamed V au Maroc, 21 July 2017, supervised by R. Aboulaich and N. Zemmendi.


PhD in progress : Y. Abidi, “Etude théorique et numérique de problème d’identification de paramètres en électrophysiologie cardiaque”. Université de Tunis El Manar, started in October 2015, supervised by M. Bellassoued and M. Mahjoub in Tunis and N. Zemmendi in Bordeaux.

9.2.3. Juries

L. Weynans: PhD comittee of Isabelle Lagrange (Onera, Toulouse), “comité de sélection” at Pau University


Y. Coudière: jury member for the PhD defense of Rémi Tesson, Université Marseille-Provence, defended December 12th, 2017.

9.3. Popularization

L. Weynans:
- Responsible for the communication (Chargé de communication) of the IMB
- Organization of the day “Filles et Maths, une équation lumineuse”
- Several presentations for high-school students about scientific computing

10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


International Conferences with Proceedings


[25] Best Paper


Conferences without Proceedings


Research Reports

[33] C. Corrado, N. Zemzemi. A conduction velocity adapted eikonal model for electrophysiology problems with re-excitability evaluation, Inria Bordeaux Sud-Ouest; King’s College London, July 2017, https://hal.inria.fr/hal-01567868.

Other Publications


[35] M. Bendahmane, E. Erraï, F. Karama. 3D Reaction-Diffusion System Describing Bidomain Calcium Dynamics in Cardiac Cell, January 2018, working paper or preprint, https://hal.inria.fr/hal-01680574.


References in notes


Project-Team CQFD

Quality control and dynamic reliability

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Stochastic approaches
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9.1.3. ANR BNPSI: Bayesian Non Parametric methods for Signal and Image Processing

9.1.4. Gaspard Monge Program for Optimisation and Operational Research (2017-2018)

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10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

10.1.2.2. Member of the Conference Program Committees

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

10.1.3.2. Reviewer - Reviewing Activities

10.1.4. Invited Talks

10.1.5. Leadership within the Scientific Community

10.1.6. Scientific Expertise

10.1.7. Research Administration

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

10.2.2. Supervision

10.2.3. Juries

11. Bibliography
Project-Team CQFD

Creation of the Project-Team: 2009 January 01

Keywords:

Computer Science and Digital Science:
A1.1.6. - Cloud
A1.2.4. - QoS, performance evaluation
A1.3. - Distributed Systems
A3.3. - Data and knowledge analysis
A3.4.1. - Supervised learning
A3.4.2. - Unsupervised learning
A3.4.5. - Bayesian methods
A3.4.6. - Neural networks
A3.4.7. - Kernel methods
A5.9.2. - Estimation, modeling
A5.9.6. - Optimization tools
A6.1.2. - Stochastic Modeling (SPDE, SDE)
A6.1.3. - Discrete Modeling (multi-agent, people centered)
A6.2.2. - Numerical probability
A6.2.3. - Probabilistic methods
A6.2.4. - Statistical methods
A6.2.6. - Optimization
A6.4.2. - Stochastic control
A8.11. - Game Theory
A9.2. - Machine learning
A9.6. - Decision support

Other Research Topics and Application Domains:
B2.2.4. - Infectious diseases, Virology
B2.6.1. - Brain imaging
B5.9. - Industrial maintenance
B6.2. - Network technologies
B6.3.3. - Network Management
B6.5. - Information systems
B9.2.3. - Video games
B9.4.2. - Mathematics

1. Personnel

Research Scientists
Jonatha Anselmi [Inria, Researcher]
Pierre Del Moral [Inria, Senior Researcher, HDR]

Faculty Members
2. Overall Objectives

2.1. Presentation

The core component of our scientific agenda focuses on the development of statistical and probabilistic methods for the modeling and the optimization of complex systems. These systems require dynamic and stochastic mathematical representations with discrete and/or continuous variables. Their complexity poses genuine scientific challenges that can be addressed through complementary approaches and methodologies:

- **Modeling:** design and analysis of realistic and tractable models for such complex real-life systems taking into account various probabilistic phenomena;
- **Estimation:** developing theoretical and computational methods in order to estimate the parameters of the model and to evaluate the performance of the system;
- **Control:** developing theoretical and numerical control tools to optimize the performance.

These three approaches are strongly connected and the most important feature of the team is to consider these topics as a whole. This enables the team to deal with real industrial problems in several contexts such as biology, production planning, trajectory generation and tracking, performance and reliability.

3. Research Program

3.1. Introduction

The scientific objectives of the team are to provide mathematical tools for modeling and optimization of complex systems. These systems require mathematical representations which are in essence dynamic, multi-model and stochastic. This increasing complexity poses genuine scientific challenges in the domain of modeling and optimization. More precisely, our research activities are focused on stochastic optimization and (parametric, semi-parametric, multidimensional) statistics which are complementary and interlinked topics. It is essential to develop simultaneously statistical methods for the estimation and control methods for the optimization of the models.
3.2. Main research topics

**Stochastic modeling**: Markov chain, Piecewise Deterministic Markov Processes (PDMP), Markov Decision Processes (MDP).

The mathematical representation of complex systems is a preliminary step to our final goal corresponding to the optimization of its performance. The team CQFD focuses on two complementary types of approaches. The first approach is based on mathematical representations built upon physical models where the dynamic of the real system is described by *stochastic processes*. The second one consists in studying the modeling issue in an abstract framework where the real system is considered as black-box. In this context, the outputs of the system are related to its inputs through a *statistical model*. Regarding stochastic processes, the team studies Piecewise Deterministic Markov Processes (PDMPs) and Markov Decision Processes (MDPs). These two classes of Markov processes form general families of controlled stochastic models suitable for the design of sequential decision-making problems. They appear in many fields such as biology, engineering, computer science, economics, operations research and provide powerful classes of processes for the modeling of complex systems. Our contribution to this topic consists in expressing real-life industrial problems into these mathematical frameworks. Regarding statistical methods, the team works on dimension reduction models. They provide a way to understand and visualize the structure of complex data sets. Furthermore, they are important tools in several different areas such as data analysis and machine learning, and appear in many applications such as biology, genetics, environment and recommendation systems. Our contribution to this topic consists in studying semiparametric modeling which combines the advantages of parametric and nonparametric models.

**Estimation methods**: estimation for PDMP; estimation in non- and semi-parametric regression modeling.

To the best of our knowledge, there does not exist any general theory for the problems of estimating parameters of PDMPs although there already exist a large number of tools for sub-classes of PDMPs such as point processes and marked point processes. To fill the gap between these specific models and the general class of PDMPs, new theoretical and mathematical developments will be on the agenda of the whole team. In the framework of non-parametric regression or quantile regression, we focus on kernel estimators or kernel local linear estimators for complete data or censored data. New strategies for estimating semi-parametric models via recursive estimation procedures have also received an increasing interest recently. The advantage of the recursive estimation approach is to take into account the successive arrivals of the information and to refine, step after step, the implemented estimation algorithms. These recursive methods do require restarting calculation of parameter estimation from scratch when new data are added to the base. The idea is to use only the previous estimations and the new data to refresh the estimation. The gain in time could be very interesting and there are many applications of such approaches.

**Dimension reduction**: dimension-reduction via SIR and related methods, dimension-reduction via multidimensional and classification methods.

Most of the dimension reduction approaches seek for lower dimensional subspaces minimizing the loss of some statistical information. This can be achieved in modeling framework or in exploratory data analysis context. In modeling framework we focus our attention on semi-parametric models in order to conjugate the advantages of parametric and nonparametric modeling. On the one hand, the parametric part of the model allows a suitable interpretation for the user. On the other hand, the functional part of the model offers a lot of flexibility. In this project, we are especially interested in the semi-parametric regression model \( Y = f(X'\theta) + \varepsilon \), the unknown parameter \( \theta \) belongs to \( \mathbb{R}^p \) for a single index model, or is such that \( \theta = [\theta_1, \ldots, \theta_d] \) (where each \( \theta_k \) belongs to \( \mathbb{R}^p \) and \( d \leq p \) for a multiple indices model), the noise \( \varepsilon \) is a random error with unknown distribution, and the link function \( f \) is an unknown real valued function. Another way to see this model is the following: the variables \( X \) and \( Y \) are independent given \( X'\theta \). In our semi-parametric framework, the main objectives are to estimate the parametric part \( \theta \) as well as the nonparametric part which can be the link function \( f \), the conditional distribution function of \( Y \) given \( X \) or the conditional quantile \( q_\alpha \). In order to estimate the dimension reduction parameter \( \theta \) we focus on the Sliced Inverse Regression (SIR) method which has been introduced by Li [53] and Duan and Li [51].
Methods of dimension reduction are also important tools in the field of data analysis, data mining and machine learning. They provide a way to understand and visualize the structure of complex data sets. Traditional methods among others are principal component analysis for quantitative variables or multiple component analysis for qualitative variables. New techniques have also been proposed to address these challenging tasks involving many irrelevant and redundant variables and often comparably few observation units. In this context, we focus on the problem of synthetic variables construction, whose goals include increasing the predictor performance and building more compact variables subsets. Clustering of variables is used for feature construction. The idea is to replace a group of "similar" variables by a cluster centroid, which becomes a feature. The most popular algorithms include K-means and hierarchical clustering. For a review, see, e.g., the textbook of Duda [52].

**Stochastic control**: optimal stopping, impulse control, continuous control, linear programming.

The main objective is to develop approximation techniques to provide quasi-optimal feasible solutions and to devise optimality results for control problems related to MDPs and PDMPs:

- **Approximation techniques.** The analysis and the resolution of such decision models mainly rely on the maximum principle and/or the dynamic/linear programming techniques together with their various extensions such as the value iteration (VIA) and the policy iteration (PIA) algorithm. However, it is well known that these approaches are hardly applicable in practice and suffer from the so-called curse of dimensionality. Hence, solving numerically a PDMP or an MDP is a difficult and important challenge. Our goal is to obtain results which are both consistent from a theoretical point of view and computationally tractable and accurate from an application standpoint. It is important to emphasize that these research objectives were not planned in our initial 2009 program.

Our objective is to propose approximation techniques to efficiently compute the optimal value function and to get quasi-optimal controls for different classes of constrained and unconstrained MDPs with general state/action spaces, and possibly unbounded cost function. Our approach is based on combining the linear programming formulation of an MDP with probabilistic approximation techniques related to quantization techniques and the theory of empirical processes. An other aim is to apply our methods to specific industrial applications in collaboration with industrial partners such as Airbus Defence & Space, DCNS and Thales.

Asymptotic approximations are also developed in the context of queueing networks, a class of models where the decision policy of the underlying MDP is in some sense fixed a priori, and our main goal is to study the transient or stationary behavior of the induced Markov process. Even though the decision policy is fixed, these models usually remain intractable to solve. Given this complexity, the team has developed analyses in some limiting regime of practical interest, i.e., queueing models in the large-network, heavy-traffic, fluid or mean-field limit. This approach is helpful to obtain a simpler mathematical description of the system under investigation, which is often given in terms of ordinary differential equations or convex optimization problems.

- **Optimality results.** Our aim is to investigate new important classes of optimal stochastic control problems including constraints and combining continuous and impulse actions for MDPs and PDMPs. In this framework, our objective is to obtain different types of optimality results. For example, we intend to provide conditions to guarantee the existence and uniqueness of the optimality equation for the problem under consideration and to ensure existence of an optimal (and \(\epsilon\)-optimal) control strategy. We also plan to analyze the structural properties of the optimal strategies as well as to study the associated infinite dimensional linear programming problem. These results can be seen as a first step toward the development of numerical approximation techniques in the sense described above.

### 4. Application Domains

#### 4.1. Dependability and safety
Our abilities in probability and statistics apply naturally to industry, in particular in studies of dependability and safety. An illustrative example is the collaboration that started in September 2014 with THALES Optronique. The goal of this project is the optimization of the maintenance of an onboard system equipped with a HUMS (Health Unit Monitoring Systems). The physical system under consideration is modeled by a piecewise deterministic Markov process. In the context of impulse control, we propose a dynamic maintenance policy, adapted to the state of the system and taking into account both random failures and those related to the degradation phenomenon.

The spectrum of applications of the topics that the team can address is large and can concern many other fields. Indeed nonparametric and semi-parametric regression methods can be used in biometry, econometrics or engineering for instance. Gene selection from microarray data and text categorization are two typical application domains of dimension reduction among others. We had for instance the opportunity via the scientific program PRIMEQUAL to work on air quality data and to use dimension reduction techniques as principal component analysis (PCA) or positive matrix factorization (PMF) for pollution sources identification and quantization.

5. Highlights of the Year

5.1. Highlights of the Year

Pierre Del Moral is a Simons foundation CRM Professor, Montréal Math. Research Center 2017


6. New Software and Platforms

6.1. biips

*Bayesian Inference with Interacting Particle Systems*

**FUNCTIONAL DESCRIPTION:** Biips is a software platform for automatic Bayesian inference with interacting particle systems. Biips allows users to define their statistical model in the probabilistic programming BUGS language, as well as to add custom functions or samplers within this language. Then it runs sequential Monte Carlo based algorithms (particle filters, particle independent Metropolis-Hastings, particle marginal Metropolis-Hastings) in a black-box manner so that to approximate the posterior distribution of interest as well as the marginal likelihood. The software is developed in C++ with interfaces with the softwares R, Matlab and Octave.

- Participants: Adrien Todeschini and François Caron
- Contact: Adrien Todeschini
- URL: [http://biips.gforge.inria.fr](http://biips.gforge.inria.fr)

6.2. PCAmixdata

**KEYWORD:** Statistic analysis
**Functional Description:** Mixed data type arise when observations are described by a mixture of numerical and categorical variables. The R package PCAmixdata extends standard multivariate analysis methods to incorporate this type of data. The key techniques included in the package are PCAmix (PCA of a mixture of numerical and categorical variables), PCArot (rotation in PCAmix) and MFAmix (multiple factor analysis with mixed data within a dataset). The MFAmix procedure handles a mixture of numerical and categorical variables within a group - something which was not possible in the standard MFA procedure. We also included techniques to project new observations onto the principal components of the three methods in the new version of the package.

- Contact: Marie Chavent
- URL: https://cran.r-project.org/web/packages/PCAmixdata/index.html

### 6.3. QuantifQuantile

**Keyword:** Regression

**Functional Description:** QuantifQuantile is an R package that allows to perform quantization-based quantile regression. The different functions of the package allow the user to construct an optimal grid of $N$ quantizers and to estimate conditional quantiles. This estimation requires a data driven selection of the size $N$ of the grid that is implemented in the functions. Illustration of the selection of $N$ is available, and graphical output of the resulting estimated curves or surfaces (depending on the dimension of the covariate) is directly provided via the plot function.

- Contact: Jérôme Saracco

### 7. New Results

#### 7.1. Asymptotically optimal open-loop load balancing

In many distributed computing systems, stochastically arriving jobs need to be assigned to servers with the objective of minimizing waiting times. Many existing dispatching algorithms are basically included in the $\text{SQ}(d)$ framework: Upon arrival of a job, $d \geq 2$ servers are contacted uniformly at random to retrieve their state and then the job is routed to a server in the best observed state. One practical issue in this type of algorithm is that server states may not be observable, depending on the underlying architecture. In [3], we investigate the assignment problem in the open-loop setting where no feedback information can flow dynamically from the queues back to the controller, i.e., the queues are unobservable. This is an intractable problem, and unless particular cases are considered, the structure of an optimal policy is not known. Under mild assumptions and in a heavy-traffic many-server limiting regime, our main result proves the optimality of a subset of deterministic and periodic policies within a wide set of (open-loop) policies that can be randomized or deterministic and can be dependent on the arrival process at the controller. The limiting value of the scaled stationary mean waiting time achieved by any policy in our subset provides a simple approximation for the optimal system performance.

Author: J. Anselmi (Inria CQFD).

#### 7.2. The economics of the cloud: price competition and congestion

The work developed in [4] proposes a model to study the interaction of price competition and congestion in the cloud computing marketplace. Specifically, we propose a three-tier market model that captures a marketplace with users purchasing services from Software-as-Service (SaaS) providers, which in turn purchase computing resources from either Provider-as-a-Service (PaaS) providers or Infrastructure-as-a-Service (IaaS) providers. Within each level, we define and characterize competitive equilibria. Further, we use these characterizations to understand the relative profitability of SaaSs and PaaSs/IaaSs, and to understand the impact of price competition on the user experienced performance, i.e., the ‘price of anarchy’ of the cloud marketplace. Our results highlight that both of these depend fundamentally on the degree to which congestion results from shared or dedicated resources in the cloud.
7.3. A new characterization of the jump rate for piecewise-deterministic Markov processes with discrete transitions

Piecewise-deterministic Markov processes form a general class of non-diffusion stochastic models that involve both deterministic trajectories and random jumps at random times. In [5], we state a new characterization of the jump rate of such a process with discrete transitions. We deduce from this result a nonparametric technique for estimating this feature of interest. We state the uniform convergence in probability of the estimator. The methodology is illustrated on a numerical example.
Authors: A. Genadot (Inria CQFD) and R. Azais.

7.4. Linear minimum mean square filters for Markov jump linear systems

In [9], new linear minimum mean square estimators are introduced by considering a cluster information structure in the filter design. The set of filters constructed in this way can be ordered in a lattice according to the refines of clusters of the Markov chain, including the linear Markovian estimator at one end (with only one cluster) and the Kalman filter at the other hand (with as many clusters as Markov states). The higher is the number of clusters, the heavier are pre-computations and smaller is the estimation error, so that the cluster cardinality allows for a trade-off between performance and computational burden. In this paper we propose the estimator, give the formulas for pre-computation of gains, present some properties, and give an illustrative numerical example.
Authors: E. Costa and B. De Saporta (Inria CQFD).

7.5. Zero-sum discounted reward criterion games for piecewise deterministic Markov processes

In [10], we deal with zero-sum games with a discounted reward criterion for piecewise deterministic Markov process (PDMPs) in general Borel spaces. The two players can act on the jump rate and transition measure of the process, with the decisions being taken just after a jump of the process. The goal of this paper is to derive conditions for the existence of minmax strategies for the infinite horizon total expected discounted reward function, which is composed of running and boundary parts. The basic idea is, by using the special features of the PDMPs, to re-write the problem via an embedded discrete-time Markov chain associated to the PDMP and re-formulate the problem as a discrete-stage zero sum game problem.
Authors: O. Costa and F. Dufour (Inria CQFD).

7.6. Optimal strategies for impulse control of piecewise deterministic Markov processes

In [11], we deal with the general discounted impulse control problem of a piecewise deterministic Markov process. We investigate a new family of optimal strategies. The construction of such strategies is explicit and only necessitates the previous knowledge of the cost of the no-impulse strategy. In particular, it does not require the resolution of auxiliary optimal stopping problem or the computation of the value function at each point of the state space. This approach is based on the iteration of a single-jump-orintervention operator associated to the piecewise deterministic Markov process.
Authors: B. De Saporta, F. Dufour and A. Geeraert. All authors are members of CQFD at Inria.
7.7. Partially observed optimal stopping problem for discrete-time Markov processes

In [12], we have investigated of a new numerical method to approximate the optimal stopping problem for a discrete-time continuous state space Markov chain under partial observations. It is based on a two-step discretization procedure based on optimal quantization. First, we discretize the state space of the unobserved variable by quantizing an underlying reference measure. Then we jointly discretize the resulting approximate filter and the observation process. We obtain a fully computable approximation of the value function with explicit error bounds for its convergence towards the true value function.

Authors: B. De Saporta, F. Dufour and C. Nivot. All authors are members of CQFD at Inria.

7.8. On the stability and the uniform propagation of chaos of a class of extended ensemble Kalman–Bucy filters

The result published in [15] deals with the exponential stability and the uniform propagation of chaos properties of a class of Extended Ensemble Kalman-Bucy filters with respect to the time horizon. This class of nonlinear filters can be interpreted as the conditional expectations of nonlinear McKean Vlasov type diffusions with respect to the observation process. In contrast with more conventional Langevin nonlinear drift type processes, the mean field interaction is encapsulated in the covariance matrix of the diffusion. The main results discussed in the article are quantitative estimates of the exponential stability properties of these nonlinear diffusions. These stability properties are used to derive uniform and non asymptotic estimates of the propagation of chaos properties of Extended Ensemble Kalman filters, including exponential concentration inequalities. To our knowledge these results seem to be the first results of this type for this class of nonlinear ensemble type Kalman-Bucy filters.

Authors: P. Del Moral (Inria CQFD), A. Kurtzmann and J. Tugaut.

7.9. Exponential mixing properties for time inhomogeneous diffusion processes with killing

In [16], we consider an elliptic and time-inhomogeneous diffusion process with time-periodic coefficients evolving in a bounded domain of \( \mathbb{R}^d \) with a smooth boundary. The process is killed when it hits the boundary of the domain (hard killing) or after an exponential time (soft killing) associated with some bounded rate function. The branching particle interpretation of the non absorbed diffusion again behaves as a set of interacting particles evolving in an absorbing medium. Between absorption times, the particles evolve independently one from each other according to the diffusion evolution operator; when a particle is absorbed, another selected particle splits into two offsprings. This article is concerned with the stability properties of these non absorbed processes. Under some classical ellipticity properties on the diffusion process and some mild regularity properties of the hard obstacle boundaries, we prove an uniform exponential strong mixing property of the process conditioned to not be killed. We also provide uniform estimates w.r.t. the time horizon for the interacting particle interpretation of these non-absorbed processes, yielding what seems to be the first result of this type for this class of diffusion processes evolving in soft and hard obstacles, both in homogeneous and non-homogeneous time settings.

Authors: P. Del Moral (Inria CQFD) and D. Villemonais.

7.10. Averaging for some simple constrained Markov processes

In [17], we study a class of piecewise deterministic Markov processes with underlying fast dynamic. Using a "penalty method" , an averaging result is obtained when the underlying dynamic is infinitely accelerated. The features of the averaged process, which is still a piecewise deterministic Markov process, are fully described.

Authors: A. Genadot (Inria CQFD).
7.11. Nonasymptotic analysis of adaptive and annealed Feynman–Kac particle models

Sequential and quantum Monte Carlo methods, as well as genetic type search algorithms can be interpreted as a mean field and interacting particle approximations of Feynman–Kac models in distribution spaces. The performance of these population Monte Carlo algorithms is strongly related to the stability properties of nonlinear Feynman–Kac semigroups. In [18], we analyze these models in terms of Dobrushin ergodic coefficients of the reference Markov transitions and the oscillations of the potential functions. Sufficient conditions for uniform concentration inequalities w.r.t. time are expressed explicitly in terms of these two quantities. We provide an original perturbation analysis that applies to annealed and adaptive Feynman-Kac models, yielding what seems to be the first results of this kind for these types of models. Special attention is devoted to the particular case of Boltzmann-Gibbs measures’ sampling. In this context, we design an explicit way of tuning the number of Markov chain Monte Carlo iterations with temperature schedule. We also design an alternative interacting particle method based on an adaptive strategy to define the temperature increments. The theoretical analysis of the performance of this adaptive model is much more involved as both the potential functions and the reference Markov transitions now depend on the random evolution on the particle model. The nonasymptotic analysis of these complex adaptive models is an open research problem. We initiate this study with the concentration analysis of a simplified adaptive models based on reference Markov transitions that coincide with the limiting quantities, as the number of particles tends to infinity.

Authors: F. Giraud and P. Del Moral (Inria CQFD).


Genetic programming (GP) is an evolutionary computation paradigm for automatic program induction. GP has produced impressive results but it still needs to overcome some practical limitations, particularly its high computational cost, overfitting and excessive code growth. Recently, many researchers have proposed fitness-case sampling methods to overcome some of these problems, with mixed results in several limited tests. In [20], we present an extensive comparative study of four fitness-case sampling methods, namely: Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and Keep-Worst Interleaved Sampling. The algorithms are compared on 11 symbolic regression problems and 11 supervised classification problems, using 10 synthetic benchmarks and 12 real-world data-sets. They are evaluated based on test performance, overfitting and average program size, comparing them with a standard GP search. Comparisons are carried out using non-parametric multigroup tests and post hoc pairwise statistical tests. The experimental results suggest that fitness-case sampling methods are particularly useful for difficult real-world symbolic regression problems, improving performance, reducing overfitting and limiting code growth. On the other hand, it seems that fitness-case sampling cannot improve upon GP performance when considering supervised binary classification.

Authors: Y. Martinez, E. Naredo, L. Trujillo, P. Legrand (Inria CQFD) and U. Lopez.

7.13. Stochastic control of observer trajectories in passive tracking with acoustic signal propagation optimization

In [23], we present a numerical method which computes the optimal trajectory of a underwater vehicle subject to some mission objectives. The method is applied to a submarine whose goal is to best detect one or several targets, or/and to minimize its own detection range perceived by the other targets. The signal considered is acoustic propagation attenuation. Our approach is based on dynamic programming of a finite horizon Markov decision process. A quantization method is applied to fully discretize the problem and allows a numerically tractable solution. Different scenarios are considered. We suppose at first that the position and the velocity of the targets are known and in the second we suppose that they are unknown and estimated by a Kalman type filter in a context of bearings-only tracking.

Authors: H. Zhang (Inria CQFD), B. De Saporta (Inria CQFD), F. Dufour (Inria CQFD), D. Laneuville and A. Nègre.
7.14. Use of local Search in Genetic Programming

There are two important limitations of standard tree-based genetic programming (GP). First, GP tends to evolve unnecessarily large programs, what is referred to as bloat. Second, GP uses inefficient search operators that focus on modifying program syntax. The first problem has been studied in many works, with many bloat control proposals. Regarding the second problem, one approach is to use alternative search operators, for instance geometric semantic operators, to improve convergence. In [36], our goal is to experimentally show that both problems can be effectively addressed by incorporating a local search optimizer as an additional search operator. Using real-world problems, we show that this rather simple strategy can improve the convergence and performance of tree-based GP, while reducing program size. Given these results, a question arises: why are local search strategies so uncommon in GP? A small survey of popular GP libraries suggests to us that local search is underused in GP systems.

Authors: Leonardo Trujillo, Emigdio Z-Flores, Perla S. Juarez Smith, Pierrick Legrand (Inria CQFD), Sara Silva, Mauro Castelli, Leonardo Vanneschi, Oliver Schutze and Luis Munoz.

7.15. Hierarchical clustering with spatial constraints

In [8], we propose a Ward-like hierarchical clustering algorithm including spatial/geographical constraints. Two dissimilarity matrices \( D_0 \) and \( D_1 \) are inputted, along with a mixing parameter \( \alpha \in [0, 1] \). The dissimilarities can be non-Euclidean and the weights of the observations can be non-uniform. The first matrix gives the dissimilarities in the "feature space" and the second matrix gives the dissimilarities in the "constraint space". The criterion minimized at each stage is a convex combination of the homogeneity criterion calculated with \( D_0 \) and the homogeneity criterion calculated with \( D_1 \). The idea is then to determine a value of \( \alpha \) which increases the spatial contiguity without deteriorating too much the quality of the solution based on the variables of interest i.e. those of the feature space. This procedure is illustrated on a real dataset using the R package ClustGeo.

Authors: Marie Chavent (Inria CQFD), Vanessa Kuentz, Amaury Labenne, Jérôme Saracco (Inria CQFD).

7.16. Variable importance assessment in sliced inverse regression for variable selection

In [19], we are interested in treating the relationship between a dependent variable \( y \) and a multivariate covariate \( x \) in a semiparametric regression model. Since the purpose of most social, biological, or environmental science research is the explanation, the determination of the importance of the variables is a major concern. It is a way to determine which variables are the most important when predicting \( y \). Sliced inverse regression methods allow to reduce the space of the covariate \( x \) by estimating the directions \( \beta \) that form an effective dimension reduction (EDR) space. The aim of this article is to propose a computational method based on important variable measure (only relying on the EDR space) in order to select the most useful variables. The numerical behavior of this new method, implemented in R, is studied on a simulation study. An illustration on a real data is also provided.

Authors: Ines Jlassi, Jérôme Saracco (Inria CQFD).

7.17. Group-sparse block PCA and explained variance

In [46], we address the simultaneous determination of group-sparse loadings by block optimization, and the correlated problem of defining explained variance for a set of non orthogonal components. We give in both cases a comprehensive mathematical presentation of the problem, which leads to propose i) a new formulation/algorithm for group-sparse block PCA and ii) a framework for the definition of explained variance with the analysis of five definitions. The numerical results i) confirm the superiority of block optimization over deflation for the determination of group-sparse loadings, and the importance of group information when available, and ii) show that ranking of algorithms according to explained variance is essentially independent of the definition of explained variance. These results lead to propose a new optimal variance as the definition of choice for explained variance.
7.18. Multivariate Analysis of Mixed Data

In [47], we focus on mixed data that arise when observations are described by a mixture of numerical and categorical variables. The R package PCAmixdata extends standard multivariate analysis methods to incorporate this type of data. The key techniques/methods included in the package are principal component analysis for mixed data (PCAmix), varimax-like orthogonal rotation for PCAmix, and multiple factor analysis for mixed multi-table data. This paper gives a synthetic presentation of the three algorithms with details to help the user understand graphical and numerical outputs of the corresponding R functions. The three main methods are illustrated on a real dataset composed of four data tables characterizing living conditions in different municipalities in the Gironde region of southwest France.

Authors: Marie Chavent (Inria CQFD), Vanessa Kuentz, Amaury Labenne, Jérôme Saracco (Inria CQFD).

7.19. A Smooth Nonparametric Estimator of a Conditional Quantile

In [50], we propose a new smooth nonparametric estimator of conditional quantile of $Y$ for a given value of $X$ using a kernel type of estimators. A numerical study to examine the performance of our estimator as well as a theoretical asymptotic study have been conducted.

Authors: Ines Jlassi, Jérôme Saracco (Inria CQFD).

7.20. Perturbations and projections of Kalman-Bucy semigroups

The purpose of the work published in [40] is to analyse the effect of various perturbations and projections of Kalman-Bucy semigroups and Riccati equations. The original motivation was to understand the behaviour of various regulation methods used in ensemble Kalman filtering (EnKF). For example, covariance inflation-type methods (perturbations) and covariance localisation methods (projections) are commonly used in the EnKF literature to ensure well-posedness of the sample covariance (e.g. sufficient rank) and to ’move’ the sample covariance closer (in some sense) to the Riccati flow of the true Kalman filter. In the limit, as the number of samples tends to infinity, these methods drive the sample covariance toward a solution of a perturbed, or projected, version of the standard (Kalman-Bucy) differential Riccati equation. The behaviour of this modified Riccati equation is investigated here. Results concerning continuity (in terms of the perturbations), boundedness, and convergence of the Riccati flow to a limit are given. In terms of the limiting filters, results characterising the error between the perturbed/projected and nominal conditional distributions are given. New projection-type models and ideas are also discussed within the EnKF framework; e.g. projections onto so-called Bose-Mesner algebras. This work is generally important in understanding the limiting bias in both the EnKF empirical mean and covariance when applying regularisation. Finally, we note the perturbation and projection models considered herein are also of interest on their own, and in other applications such as differential games, control of stochastic and jump processes, and robust control theory, etc.

Authors: Pierre Del Moral (Inria CQFD), Adrian Bishop and Sahani Pathiraja.

7.21. Probabilistic Safety Analysis of the Collision Between a Space Debris and a Satellite with an Island Particle Algorithm

Collision between satellites and space debris seldom happens, but the loss of a satellite by collision may have catastrophic consequences both for the satellite mission and for the space environment. To support the decision to trigger a collision avoidance manoeuvre, an adapted tool is the determination of the collision probability between debris and satellite. This probability estimation can be performed with rare event simulation techniques when Monte Carlo techniques are not enough accurate. In this chapter, we focus on analyzing the influence of different simulation parameters (such as the drag coefficient) that are set for to simplify the simulation, on the collision probability estimation. A bad estimation of these simulation parameters can strongly modify rare event probability estimations. We design here a new island particle Markov chain Monte
Carlo algorithm to determine the parameters that, in case of bad estimation, tend to increase the collision probability value. This algorithm also gives an estimate of the collision probability maximum taking into account the likelihood of the parameters. The principles of this statistical technique are described throughout this chapter.

Authors: Pierre Del Moral (Inria CQFD), Christelle Vergé, Jérôme Morio and Juan Carlos Dolado Pérez.

7.22. Biased online parameter inference for state-space models

We consider Bayesian online static parameter estimation for state-space models. This is a very important problem, but is very computationally challenging as the state-of-the art methods that are exact, often have a computational cost that grows with the time parameter; perhaps the most successful algorithm is that of SM C2 (Chopin et al., J R Stat Soc B 75: 397–426 2013). We present a version of the SM C2 algorithm which has computational cost that does not grow with the time parameter. In addition, under assumptions, the algorithm is shown to provide consistent estimates of expectations w.r.t. the posterior. However, the cost to achieve this consistency can be exponential in the dimension of the parameter space; if this exponential cost is avoided, typically the algorithm is biased. The bias is investigated from a theoretical perspective and, under assumptions, we find that the bias does not accumulate as the time parameter grows. The algorithm is implemented on several Bayesian statistical models.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Yan Zhou.

7.23. Multilevel Sequential Monte Carlo Samplers for Normalizing Constants

This work considers the sequential Monte Carlo (SMC) approximation of ratios of normalizing constants associated to posterior distributions which in principle rely on continuum models. Therefore, the Monte Carlo estimation error and the discrete approximation error must be balanced. A multilevel strategy is utilized to substantially reduce the cost to obtain a given error level in the approximation as compared to standard estimators. Two estimators are considered and relative variance bounds are given. The theoretical results are numerically illustrated for the example of identifying a parametrized permeability in an elliptic equation given point-wise observations of the pressure.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra, Kody Law and Yan Zhou.

7.24. Multilevel sequential Monte Carlo: Mean square error bounds under verifiable conditions

In this article, we consider the multilevel sequential Monte Carlo (MLSMC) method of Beskos et al. (Stoch. Proc. Appl. [to appear]). This is a technique designed to approximate expectations w.r.t. probability laws associated to a discretization. For instance, in the context of inverse problems, where one discretizes the solution of a partial differential equation. The MLMC approach is especially useful when independent, coupled sampling is not possible. Beskos et al. show that for MLMC the computational effort to achieve a given error, can be less than independent sampling. In this article we significantly weaken the assumptions of Beskos et al., extending the proofs to non-compact state-spaces. The assumptions are based upon multiplicative drift conditions as in Kontoyiannis and Meyn (Electron. J. Probab. 10 [2005]: 61–123). The assumptions are verified for an example.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Kody Law.

7.25. Biased Online Parameter Inference for State-Space Models

We consider Bayesian online static parameter estimation for state-space models. This is a very important problem, but is very computationally challenging as the state-of-the art methods that are exact, often have a computational cost that grows with the time parameter; perhaps the most successful algorithm is that of SM C2 (Chopin et al., J R Stat Soc B 75: 397–426 2013). We present a version of the SM C2 algorithm
which has computational cost that does not grow with the time parameter. In addition, under assumptions, the algorithm is shown to provide consistent estimates of expectations w.r.t. the posterior. However, the cost to achieve this consistency can be exponential in the dimension of the parameter space; if this exponential cost is avoided, typically the algorithm is biased. The bias is investigated from a theoretical perspective and, under assumptions, we find that the bias does not accumulate as the time parameter grows. The algorithm is implemented on several Bayesian statistical models.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Yan Zhou.

7.26. Valuation of Barrier Options using Sequential Monte Carlo

Sequential Monte Carlo (SMC) methods have successfully been used in many applications in engineering, statistics and physics. However, these are seldom used in financial option pricing literature and practice. This paper presents SMC method for pricing barrier options with continuous and discrete monitoring of the barrier condition. Under the SMC method, simulated asset values rejected due to barrier condition are re-sampled from asset samples that do not breach the barrier condition improving the efficiency of the option price estimator; while under the standard Monte Carlo many simulated asset paths can be rejected by the barrier condition making it harder to estimate option price accurately. We compare SMC with the standard Monte Carlo method and demonstrate that the extra effort to implement SMC when compared with the standard Monte Carlo is very little while improvement in price estimate can be significant. Both methods result in unbiased estimators for the price converging to the true value as \(1/\sqrt{M}\), where \(M\) is the number of simulations (asset paths). However, the variance of SMC estimator is smaller and does not grow with the number of time steps when compared to the standard Monte Carlo. In this paper we demonstrate that SMC can successfully be used for pricing barrier options. SMC can also be used for pricing other exotic options and also for cases with many underlying assets and additional stochastic factors such as stochastic volatility; we provide general formulas and references.

Authors: Pierre Del Moral (Inria CQFD) and Pavel V. Shevchenko.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. DCNS

Participants: Huilong Zhang, Jonatha Anselmi, François Dufour, Dann Laneuville.

The increasing complexity of warfare submarine missions has led DCNS to study new tactical help functions for underwater combat management systems. In this context, the objective is to find optimal trajectories according to the current mission type by taking into account sensors, environment and surrounding targets. This problem has been modeled as a discrete-time Markov decision process with finite horizon. A quantization technique has been applied to discretize the problem in order to get a finite MDP for which standard methods such as the dynamic and/or the linear programming approaches can be applied. Different kind of scenarios have been considered and studied.

8.1.2. Thales Optronique

Participants: Benoîte de Saporta, François Dufour, Alizée Geeraert.

Maintenance, impulse control, failure, optimization. The objective of this grant in collaboration with Thales Optronique was to optimize the maintenance of a multi-component equipment that can break down randomly. The underlying problem was to choose the best dates to repair or replace components in order to minimize a cost criterion that takes into account costs of maintenance but also the cost associated to the unavailability of the system for the customer. This industrial process has been modeled by a piecewise deterministic Markov process (PDMP) and the maintenance problem has been formalized as an impulse control problem. We have
applied an approximation method based on a quantization technique of the post jump location and inter-arrival time Markov chain naturally embedded in the PDMP, and a path-adapted time discretization grids to get an approximation of the value function. We have shown the existence of control strategies that can outperform reference control policies used by Thales Optronique. It remains to provide the explicit form of such strategies. This is actually the objective of a new collaboration with Thales Optronique that started in October 2017 funded by the Fondation Mathématique Jacques Hadamard.

8.1.3. Lyre: ADEQWAT project
Participants: François Dufour, Alexandre Genadot, Jérôme Saracco.

Stochastic modelling, Optimization. This project has just started in November 2017. The topic of this collaboration with Lyre, l’Agence de l’eau Adour-Garonne and ENSEGID is the modeling of the uncertainties in the Water demand adequacy in a context of global climate change. A PhD thesis (2018-2021) is part of this project.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR Piece (2013-2017) of the program Jeunes chercheuses et jeunes chercheurs of the ANR

Piecewise Deterministic Markov Processes (PDMP) are non-diffusive stochastic processes which naturally appear in many areas of applications as communication networks, neuron activities, biological populations or reliability of complex systems. Their mathematical study has been intensively carried out in the past two decades but many challenging problems remain completely open. This project aims at federating a group of experts with different backgrounds (probability, statistics, analysis, partial derivative equations, modelling) in order to pool everyone’s knowledge and create new tools to study PDMPs. The main lines of the project relate to estimation, simulation and asymptotic behaviors (long time, large populations, multi-scale problems) in the various contexts of application.

9.1.2. ANR StocMC (2014-2018) of the program Project Blanc of the ANR

The involved research groups are Inria Rennes/IRISA Team SUMO; Inria Rocquencourt Team Lifeware; LIAFA University Paris 7; Bordeaux University.
The aim of this research project is to develop scalable model checking techniques that can handle large stochastic systems. Large stochastic systems arise naturally in many different contexts, from network systems to system biology. A key stochastic model we will consider is from the biological pathway of apoptosis, the programmed cell death.

9.1.3. ANR BNPSI: Bayesian Non Parametric methods for Signal and Image Processing

Statistical methods have become more and more popular in signal and image processing over the past decades. These methods have been able to tackle various applications such as speech recognition, object tracking, image segmentation or restoration, classification, clustering, etc. We propose here to investigate the use of Bayesian nonparametric methods in statistical signal and image processing. Similarly to Bayesian parametric methods, this set of methods is concerned with the elicitation of prior and computation of posterior distributions, but now on infinite-dimensional parameter spaces. Although these methods have become very popular in statistics and machine learning over the last 15 years, their potential is largely underexploited in signal and image processing. The aim of the overall project, which gathers researchers in applied probabilities, statistics, machine learning and signal and image processing, is to develop a new framework for the statistical signal and image processing communities. Based on results from statistics and machine learning we aim at defining new models, methods and algorithms for statistical signal and image processing. Applications to hyperspectral image analysis, image segmentation, GPS localization, image restoration or space-time tomographic reconstruction will allow various concrete illustrations of the theoretical advances and validation on real data coming from realistic contexts.
9.1.4. Gaspard Monge Program for Optimisation and Operational Research (2017-2018)

The involved research groups are Inria Bordeaux Sud-Ouest Team CQFD and Thales Optronique. This new collaboration with Thales Optronique that started in October 2017 is funded by the Fondation Mathématique Jacques Hadamard. This is the continuation of the PhD Thesis of A. Geeraert. The objective of this project is to optimize the maintenance of a multi-component equipment that can break down randomly. The underlying problem is to choose the best dates to repair or replace components in order to minimize a cost criterion that takes into account costs of maintenance but also the cost associated to the unavailability of the system for the customer. In the PhD thesis of A. Geeraert, the model under consideration was rather simple and only a numerical approximation of the value function was provided. Here, our objective is more ambitious. A more realistic model will be considered and our aim is to provide a tractable quasi-optimal control strategy that can be applied in practice to optimize the maintenance of such equipments.

9.2. European Initiatives

9.2.1. Collaborations in European Programs, Except FP7 & H2020

- Program: Direcion General de Investigacion Cientifica y Tecnica, Gobierno de Espana
- Project acronym: GAMECONAPX
- Project title: Numerical approximations for Markov decision processes and Markov games
- Duration: 01/2017 - 12/2019
- Coordinator: Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED (Spain)
- Abstract:

This project is funded by the Gobierno de Espana, Direcion General de Investigacion Cientifica y Tecnica (reference number: MTM2016-75497-P) for three years to support the scientific collaboration between Tomas Prieto-Rumeau, Jonatha Anselmi and Francois Dufour. This research project is concerned with numerical approximations for Markov decision processes and Markov games. Our goal is to propose techniques allowing to approximate numerically the optimal value function and the optimal strategies of such problems. Although such decision models have been widely studied theoretically and, in general, it is well known how to characterize their optimal value function and their optimal strategies, the explicit calculation of these optimal solutions is not possible except for a few particular cases. This shows the need for numerical procedures to estimate or to approximate the optimal solutions of Markov decision processes and Markov games, so that the decision maker can really have at hand some approximation of his optimal strategies and his optimal value function. This project will explore areas of research that have been, so far, very little investigated. In this sense, we expect our techniques to be a breakthrough in the field of numerical methods for continuous-time Markov decision processes, but particularly in the area of numerical methods for Markov game models. Our techniques herein will cover a wide range of models, including discrete- and continuous-time models, problems with unbounded cost and transition rates, even allowing for discontinuities of these rate functions. Our research results will combine, on one hand, mathematical rigor (with the application of advanced tools from probability and measure theory) and, on the other hand, computational efficiency (providing accurate and ?applicable? numerical methods). In this sense, particular attention will be paid to models of practical interest, including population dynamics, queueing systems, or birth-and-death processes, among others. So, we expect to develop a generic and robust methodology in which, by suitably specifying the data of the decision problem, an algorithm will provide the approximations of the value function and the optimal strategies. Therefore, the results that we intend to obtain in this research project will be of interest for researchers in the fields of Markov decision processes and Markov games, both for the theoretical and the applied or practitioners communities.
9.3. International Initiatives

9.3.1. Inria International Partners

9.3.1.1. Declared Inria International Partners

**Tree-Lab, ITT.** TREE-LAB is part of the Cybernetics research line within the Engineering Science graduate program offered by the Department of Electric and Electronic Engineering at Tijuana’s Institute of Technology (ITT), in Tijuana Mexico. TREE-LAB is mainly focused on scientific and engineering research within the intersection of broad scientific fields, particularly Computer Science, Heuristic Optimization and Pattern Analysis. In particular, specific domains studied at TREE-LAB include Genetic Programming, Classification, Feature Based Recognition, Bio-Medical signal analysis and Behavior-Based Robotics. Currently, TREE-LAB incorporates the collaboration of several top researchers, as well as the participation of graduate (doctoral and masters) and undergraduate students, from ITT. Moreover, TREE-LAB is actively collaborating with top researchers from around the world, including Mexico, France, Spain, Portugal and USA.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

Tomas Prieto-Rumeau (Department of Statistics and Operations Research, UNED, Madrid, Spain) visited the team during 2 weeks in 2017. The main subject of the collaboration is the approximation of Markov Decision Processes.

Oswaldo Costa (Escola Politécnica da Universidade de São Paulo, Brazil) collaborate with the team on the theoretical aspects of continuous control of piecewise-deterministic Markov processes. He visited the team during two weeks in 2017.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

P. Legrand was co-organizer of EA 2017.

F. Dufour has been a member of the Organizing Committee of the SIAM Conference on Control and Its Applications (CT17) in Pittsburgh, USA, 2017.

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

P. Legrand was chair for EA 2017.

10.1.2.2. Member of the Conference Program Committees

J. Anselmi has been a member of the TPC of the following international conferences: VALUETOOLS-2017, ASMTA-2017 and IFIP Performance 2017.

P. Legrand has been a member of the PC of the following international conferences: EA 2017.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

P. Del Moral is an associate editor for the journal Stochastic Analysis and Applications since 2001.

P. Del Moral is an associate editor for the journal Revista de Matematica: Teoria y aplicaciones since 2009.
P. Del Moral is an associate editor for the journal Applied Mathematics and Optimization since 2009.
F. Dufour is associate editor of the journal: SIAM Journal of Control and Optimization since 2009.
F. Dufour is the representative of the SIAM activity group in control and system theory for the journal SIAM News since 2014.

10.1.3.2. Reviewer - Reviewing Activities
All the members of CQFD are regular reviewers for several international journals and conferences in applied probability, statistics and operations research.

10.1.4. Invited Talks
Pierrick Legrand was invited to give a talk on IA in Thales center in october.
Pierre del Moral gave several invited talks listed at the following address: http://people.bordeaux.inria.fr/pierre.delmoral/conf.html

10.1.5. Leadership within the Scientific Community
P. Legrand was the scientific leader of the programs HUMO 3 (with UBX and IMS) and MICRO-DOPPLER (with Thales and IMS) in the context of the GIS ALBATROS.

10.1.6. Scientific Expertise
Pierrick Legrand has been reviewer for the ANR generics projects in 2017.
J. Saracco is elected member of the council of the Société Française de Statistique (SFdS, French Statistical Society).
J. Saracco was vice president of SFdS from 2014 to 2016.

10.1.7. Research Administration
J. Saracco is deputy director of IMB (Institut de Mathématiques de Bordeaux, UMR CNRS 5251) since 2015.
M. Chavent is member of the national evaluation committee of Inria.
M. Chavent and Pierrick Legrand are members of the council of the Institut de Mathématique de Bordeaux.
Pierrick Legrand was the director of the Ressources Center Victoire of the UF Mathematics and interactions until may 2017.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching
- Licence: M. Chavent, Analyse des données, 15 ETD, L3, Bordeaux university, France
- License: M. Chavent, Modélisation statistique, 15 ETD, niveau L3, Bordeaux university, France
- Master : M. Chavent, Apprentissage automatique, 50 ETD, niveau M2, Bordeaux university, France
- Licence : F. Dufour, Probabilités et statistiques, 70h, first year of école ENSEIRB-MATMECA, Institut Polytechnique de Bordeaux, France.
• Master : F. Dufour, Méthodes numériques pour la fiabilité, 36h, third year of école ENSEIRB-MATMECA, Institut Polytechnique de Bordeaux, France.
• P. Legrand, Algèbre (responsable de l’UE), Licence 1 SCIMS (108 heures)
• P. Legrand, Informatique pour les mathématiques (responsable de l’UE), Licence 1 et Licence 2 (36 heures)
• P. Legrand, Espaces Euclidiens. (responsable de l’UE), Licence 2 SCIMS (54 heures)
• Licence: J. Saracco, Probability and Descriptive statistics, 27h, L3, First year of ENSC - Bordeaux INP, France
• Licence: J. Saracco, Mathematical statistics, 20h, L3, First year of ENSC - Bordeaux INP, France
• Licence: J. Saracco, Data analysis (multidimensional statistics), 20h, L3, First year of ENSC - Bordeaux INP, France
• Master: J. Saracco, Statistical modeling, 27h, M1, Second year of ENSC - Bordeaux INP, France
• Master: J. Saracco, Applied probability and Statistics, 40h, M1, Second year of ENSCBP - Bordeaux INP, France
• Master: J. Saracco, Probability and Statistics, 12h, M2, Science Po Bordeaux, France
• A. Genadot, Probabilités de bases (18h), Licence MIASHS première année, Université de Bordeaux.
• A. Genadot, Statistiques de bases (18h), Licence MIASHS première année, Université de Bordeaux.
• A. Genadot, Probabilités (36h), Licence MIASHS deuxième année, Université de Bordeaux.
• A. Genadot, Processus (18h), Licence MIASHS troisième année, Université de Bordeaux.
• A. Genadot, Modélisation statistique (18h), Licence MIASHS troisième année, Université de Bordeaux.
• A. Genadot, Martingales (25h), Master MIMSE première année, Université de Bordeaux.
• A. Genadot, Probabilités (20h), Master MEEF première année, Université de Bordeaux.

10.2.2. Supervision
• PhD completed : Alizé Geeraert, Contrôle optimal des processus Markoviens déterministes par morceaux et application à la maintenance, University of Bordeaux, supervised by B. de Saporta and F. Dufour (defense in June 2017).
• PhD in progress : Ines Jlassi, Contributions à la régression inverse par tranches et à l’estimation non para métrique des quantiles conditionnels, University of Monastir (Tunisia), September 2013, supervised by J. Saracco and L. Ben Abdelghani Bouraoui.
• PhD in progress : Hadrien Lorenzo, Analyses de données longitudinales de grandes dimensions appliquées aux essais vaccinaux contre le VIH et Ebola, University of Bordeaux, September 2016, supervised by J. Saracco and R. Thiebaut.
• PhD in progress : Tiffany Cherchi, “Automated optimal fleet management policy for airborne equipment”, Montpellier University, since 2017, supervised by B. De Saporta and F. Dufour.
• PhD in progress : Maud Joubaud, “Branching piecewise deterministic Markov processes, applications to cell biology”, Montpellier University, since 2016, supervised by B. De Saporta and B. Cloez.

10.2.3. Juries

J. Saracco is vice president of the french statistical society (SFdS).
11. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


Articles in National Peer-Reviewed Journal


Invited Conferences


International Conferences with Proceedings


Conferences without Proceedings


Scientific Books (or Scientific Book chapters)


Research Reports


Other Publications


[43] R. Azaïs, A. Genadot, B. Henry. Inference for conditioned Galton-Watson trees from their Harris path, June 2017, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01360650.


References in notes


Project-Team FLOWERS

Flowing Epigenetic Robots and Systems

IN PARTNERSHIP WITH:
Ecole nationale supérieure des techniques avancées

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Robotics and Smart environments
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Project-Team FLOWERS

Creation of the Team: 2008 April 01, updated into Project-Team: 2011 January 01

Keywords:

Computer Science and Digital Science:
- A5.1.1. - Engineering of interactive systems
- A5.1.2. - Evaluation of interactive systems
- A5.1.4. - Brain-computer interfaces, physiological computing
- A5.1.5. - Body-based interfaces
- A5.1.6. - Tangible interfaces
- A5.1.7. - Multimodal interfaces
- A5.3.3. - Pattern recognition
- A5.4.1. - Object recognition
- A5.4.2. - Activity recognition
- A5.7.3. - Speech
- A5.8. - Natural language processing
- A5.10.5. - Robot interaction (with the environment, humans, other robots)
- A5.10.7. - Learning
- A5.10.8. - Cognitive robotics and systems
- A5.11.1. - Human activity analysis and recognition
- A6.3.1. - Inverse problems
- A9. - Artificial intelligence
- A9.2. - Machine learning
- A9.5. - Robotics
- A9.7. - AI algorithmics

Other Research Topics and Application Domains:
- B1.2.1. - Understanding and simulation of the brain and the nervous system
- B1.2.2. - Cognitive science
- B5.6. - Robotic systems
- B5.7. - 3D printing
- B5.8. - Learning and training
- B9. - Society and Knowledge
- B9.1. - Education
- B9.1.1. - E-learning, MOOC
- B9.2. - Art
- B9.2.1. - Music, sound
- B9.2.4. - Theater
- B9.5. - Humanities
- B9.5.1. - Psychology
- B9.5.8. - Linguistics
- B9.7. - Knowledge dissemination
1. Personnel

Research Scientists
- Pierre-Yves Oudeyer [Team leader, Inria, Senior Researcher, HDR]
- Olivier Sigaud [Inria, Senior Researcher, from Sep 2017, HDR]
- Anna-Lisa Vollmer [Inria, Starting Research Position, until Feb 2017]

Faculty Member
- David Filliat [École Nationale Supérieure de Techniques Avancées, Professor, HDR]

Technical Staff
- Natalia Diaz Rodriguez [Armines]
- Yoan Mollard [Inria, until Nov 2017, granted by FP7/13-3RDHAND project]
- Stephanie Noirpoudre [Inria]
- Alexandre Pere [Inria, from Oct 2017]
- Didier Roy [Inria, granted by Bibliothèques sans frontières]
- Theo Segonds [Inria]
- Damien Caselli [Inria]

PhD Students
- Baptiste Busch [Inria]
- Benjamin Clement [Inria]
- Cedric Colas [Inria, from Nov 2017]
- Céline Craye [Thales, until Mar 2017]
- Alexandra Delmas [ITWell]
- Thibault Desprez [Inria]
- Sébastien Forestier [Univ de Bordeaux]
- Florian Golemo [Inria]
- Antonin Raffin [Ensta]
- Timothee Lesort [Ensta]
- Adrien Matricon [Univ de Bordeaux, until Nov 2017]
- Alvaro Ovalle Castaneda [Inria, until Aug 2017]
- Gennaro Raiola [École Nationale Supérieure de Techniques Avancées, until Jan 2017]
- William Schueller [Univ de Bordeaux]

Post-Doctoral Fellow
- Adrien Laversanne-Finot [Inria, from Nov 2017]

Administrative Assistants
- Nathalie Robin [Inria]
- Catherine Cattaert Megrat [Inria]

2. Overall Objectives

2.1. Overall Objectives

Can a robot learn like a child? Can it learn new skills and new knowledge in an unknown and changing environment? How can it discover its body and its relationships with the physical and social environment? How can its cognitive capacities continuously develop without the intervention of an engineer? What can it learn through natural social interactions with humans?
These are the questions that are being investigated in the FLOWERS research team at Inria Bordeaux Sud-Ouest. Rather than trying to imitate the intelligence of adult humans like in the field of Artificial Intelligence, we believe that trying to reconstruct the processes of development of the child’s mind will allow for more adaptive, more robust and more versatile machines. This approach is called developmental robotics, or epigenetic robotics, and imports concepts and theories from developmental psychology. As most of these theories are not formalized, this implies a crucial computational modeling activity, which in return provides means to assess the internal coherence of theories and sketch new hypothesis about the development of the human child’s sensorimotor and cognitive abilities.

Our team focuses in particular on the study of developmental constraints that allow for efficient open-ended learning of novel sensorimotor and interaction skills in embodied systems. In particular, we study constraints that guide exploration in large sensorimotor spaces:

- Mechanisms of intrinsically motivated exploration and active learning, including artificial curiosity, allowing in particular to self-organize developmental trajectories and collect efficiently learning data;
- Mechanisms of adequately constrained optimization and statistical inference for sensorimotor skill acquisition (e.g. for optimizing motor policies in real robots);
- Mechanisms for social learning, e.g. learning by imitation or demonstration, which implies both issues related to machine learning and human-robot interaction;
- Constraints related to embodiment, in particular through the concept of morphological computation, as well as the structure of motor primitives/muscle synergies that can leverage the properties of morphology and physics for simplifying motor control and perception;
- Maturational constraints which, coupled with the other constraints, can allow the progressive release of novel sensorimotor degrees of freedom to be explored;

We also study how these constraints on exploration can allow a robot to bootstrap multimodal perceptual abstractions associated to motor skills, in particular in the context of modelling language acquisition as a developmental process grounded in action.

Among the developmental principles that characterize human infants and can be used in developmental robots, FLOWERS focuses on the following three principles:

- **Exploration is progressive.** The space of skills that can be learnt in real world sensorimotor spaces is so large and complicated that not everything can be learnt at the same time. Simple skills are learnt first, and only when they are mastered, new skills of progressively increasing difficulty become the behavioural focus;
- **Internal representations are (partially) not innate but learnt and adaptive.** For example, the body map, the distinction self/non-self and the concept of “object” are discovered through experience with initially uninterpreted sensors and actuators, guided by experience, the overall pre-determined connection structure of the brain, as well as a small set of simple innate values or preferences.
- **Exploration can be self-guided and/or socially guided.** On the one hand, internal and intrinsic motivation systems regulate and organize spontaneous exploration; on the other hand, exploration can be guided through social learning and interaction with caretakers.

### 2.1.1. Research axis

The work of FLOWERS is organized around the following axis:

- **Curiosity-driven exploration and sensorimotor learning:** intrinsic motivation are mechanisms that have been identified by developmental psychologists to explain important forms of spontaneous exploration and curiosity. In FLOWERS, we try to develop computational intrinsic motivation systems, and test them on robots, allowing to regulate the growth of complexity in exploratory behaviours. These mechanisms are studied as active learning mechanisms, allowing to learn efficiently in large inhomogeneous sensorimotor spaces;
• **Cumulative learning of sensorimotor skills**: FLOWERS develops machine learning algorithms that can allow embodied machines to acquire cumulatively sensorimotor skills. In particular, we develop optimization and reinforcement learning systems which allow robots to discover and learn dictionaries of motor primitives, and then combine them to form higher-level sensorimotor skills.

• **Natural and intuitive social learning**: FLOWERS develops interaction frameworks and learning mechanisms allowing non-engineer humans to teach a robot naturally. This involves two sub-themes: 1) techniques allowing for natural and intuitive human-robot interaction, including simple ergonomic interfaces for establishing joint attention; 2) learning mechanisms that allow the robot to use the guidance hints provided by the human to teach new skills;

• **Discovering and abstracting the structure of sets of uninterpreted sensors and motors**: FLOWERS studies mechanisms that allow a robot to infer structural information out of sets of sensorimotor channels whose semantics is unknown, for example the topology of the body and the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations to abstract concepts and categories similar to those used by humans.

• **Body design and role of the body in sensorimotor and social development**: We study how the physical properties of the body (geometry, materials, distribution of mass, growth, ...) can impact the acquisition of sensorimotor and interaction skills. This requires to consider the body as an experimental variable, and for this we develop special methodologies for designing and evaluating rapidly new morphologies, especially using rapid prototyping techniques like 3D printing.

• **Intelligent Tutoring Systems**: FLOWERS develops methods for online personalization of teaching sequences for educational software and MOOCs. This work builds on top of online optimization methods and motivational research previously developed.

### 3. Research Program

#### 3.1. Research Program

Research in artificial intelligence, machine learning and pattern recognition has produced a tremendous amount of results and concepts in the last decades. A blooming number of learning paradigms - supervised, unsupervised, reinforcement, active, associative, symbolic, connectionist, situated, hybrid, distributed learning... - nourished the elaboration of highly sophisticated algorithms for tasks such as visual object recognition, speech recognition, robot walking, grasping or navigation, the prediction of stock prices, the evaluation of risk for insurances, adaptive data routing on the internet, etc... Yet, we are still very far from being able to build machines capable of adapting to the physical and social environment with the flexibility, robustness, and versatility of a one-year-old human child.

Indeed, one striking characteristic of human children is the nearly open-ended diversity of the skills they learn. They not only can improve existing skills, but also continuously learn new ones. If evolution certainly provided them with specific pre-wiring for certain activities such as feeding or visual object tracking, evidence shows that there are also numerous skills that they learn smoothly but could not be “anticipated” by biological evolution, for example learning to drive a tricycle, using an electronic piano toy or using a video game joystick. On the contrary, existing learning machines, and robots in particular, are typically only able to learn a single pre-specified task or a single kind of skill. Once this task is learnt, for example walking with two legs, learning is over. If one wants the robot to learn a second task, for example grasping objects in its visual field, then an engineer needs to re-program manually its learning structures: traditional approaches to task-specific machine/robot learning typically include engineer choices of the relevant sensorimotor channels, specific design of the reward function, choices about when learning begins and ends, and what learning algorithms and associated parameters shall be optimized.
As can be seen, this requires a lot of important choices from the engineer, and one could hardly use the term "autonomous" learning. On the contrary, human children do not learn following anything looking like that process, at least during their very first years. Babies develop and explore the world by themselves, focusing their interest on various activities driven both by internal motives and social guidance from adults who only have a folk understanding of their brains. Adults provide learning opportunities and scaffolding, but eventually young babies always decide for themselves what activity to practice or not. Specific tasks are rarely imposed to them. Yet, they steadily discover and learn how to use their body as well as its relationships with the physical and social environment. Also, the spectrum of skills that they learn continuously expands in an organized manner: they undergo a developmental trajectory in which simple skills are learnt first, and skills of progressively increasing complexity are subsequently learnt.

A link can be made to educational systems where research in several domains have tried to study how to provide a good learning experience to learners. This includes the experiences that allow better learning, and in which sequence they must be experienced. This problem is complementary to that of the learner that tries to learn efficiently, and the teacher here has to use as efficiently the limited time and motivational resources of the learner. Several results from psychology [100] and neuroscience [22] have argued that the human brain feels intrinsic pleasure in practicing activities of optimal difficulty or challenge. A teacher must exploit such activities to create positive psychological states of flow [111].

A grand challenge is thus to be able to build robotic machines that possess this capability to discover, adapt and develop continuously new know-how and new knowledge in unknown and changing environments, like human children. In 1950, Turing wrote that the child’s brain would show us the way to intelligence: “Instead of trying to produce a program to simulate the adult mind, why not rather try to produce one which simulates the child’s” [173]. Maybe, in opposition to work in the field of Artificial Intelligence who has focused on mechanisms trying to match the capabilities of "intelligent" human adults such as chess playing or natural language dialogue [123], it is time to take the advice of Turing seriously. This is what a new field, called developmental (or epigenetic) robotics, is trying to achieve [141] [178]. The approach of developmental robotics consists in importing and implementing concepts and mechanisms from developmental psychology [145], cognitive linguistics [110], and developmental cognitive neuroscience [128] where there has been a considerable amount of research and theories to understand and explain how children learn and develop. A number of general principles are underlying this research agenda: embodiment [104] [153], grounding [121], situatedness [91], self-organization [169] [155], enaction [176], and incremental learning [107].

Among the many issues and challenges of developmental robotics, two of them are of paramount importance: exploration mechanisms and mechanisms for abstracting and making sense of initially unknown sensorimotor channels. Indeed, the typical space of sensorimotor skills that can be encountered and learnt by a developmental robot, as those encountered by human infants, is immensely vast and inhomogeneous. With a sufficiently rich environment and multimodal set of sensors and effectors, the space of possible sensorimotor activities is simply too large to be explored exhaustively in any robot’s life time: it is impossible to learn all possible skills and represent all conceivable sensory percepts. Moreover, some skills are very basic to learn, some other very complicated, and many of them require the mastery of others in order to be learnt. For example, learning to manipulate a piano toy requires first to know how to move one’s hand to reach the piano and how to touch specific parts of the toy with the fingers. And knowing how to move the hand might require to know how to track it visually.

Exploring such a space of skills randomly is bound to fail or result at best on very inefficient learning [150]. Thus, exploration needs to be organized and guided. The approach of epigenetic robotics is to take inspiration from the mechanisms that allow human infants to be progressively guided, i.e. to develop. There are two broad classes of guiding mechanisms which control exploration:

1. **internal guiding mechanisms**, and in particular intrinsic motivation, responsible of spontaneous exploration and curiosity in humans, which is one of the central mechanisms investigated in FLOWERS, and technically amounts to achieve online active self-regulation of the growth of complexity in learning situations;

2. **social learning and guidance**, a learning mechanisms that exploits the knowledge of other agents
in the environment and/or that is guided by those same agents. These mechanisms exist in many
different forms like emotional reinforcement, stimulus enhancement, social motivation, guidance,
feedback or imitation, some of which being also investigated in FLOWERS;

3.1.1. Internal guiding mechanisms

In infant development, one observes a progressive increase of the complexity of activities with an associated
progressive increase of capabilities [145], children do not learn everything at one time: for example, they first
learn to roll over, then to crawl and sit, and only when these skills are operational, they begin to learn how to
stand. The perceptual system also gradually develops, increasing children perceptual capabilities other time
while they engage in activities like throwing or manipulating objects. This make it possible to learn to identify
objects in more and more complex situations and to learn more and more of their physical characteristics.

Development is therefore progressive and incremental, and this might be a crucial feature explaining the
efficiency with which children explore and learn so fast. Taking inspiration from these observations, some
roboticists and researchers in machine learning have argued that learning a given task could be made much
easier for a robot if it followed a developmental sequence and “started simple” [95] [114]. However, in these
experiments, the developmental sequence was crafted by hand: roboticists manually build simpler versions of
a complex task and put the robot successively in versions of the task of increasing complexity. And when they
wanted the robot to learn a new task, they had to design a novel reward function.

Thus, there is a need for mechanisms that allow the autonomous control and generation of the developmental
trajectory. Psychologists have proposed that intrinsic motivations play a crucial role. Intrinsic motivations
are mechanisms that push humans to explore activities or situations that have intermediate/optimal levels of
novelty, cognitive dissonance, or challenge [100] [111] [113]. The role and structure of intrinsic motivation in
humans have been made more precise thanks to recent discoveries in neuroscience showing the implication of
dopaminergic circuits and in exploration behaviours and curiosity [112] [125] [164]. Based on this, a number
of researchers have began in the past few years to build computational implementation of intrinsic motivation
[150] [151] [162] [99] [126] [143] [163]. While initial models were developed for simple simulated worlds,
a current challenge is to manage to build intrinsic motivation systems that can efficiently drive exploratory
behaviour in high-dimensional unprepared real world robotic sensorimotor spaces [151], [150], [152], [161].
Specific and complex problems are posed by real sensorimotor spaces, in particular due to the fact that they
are both high-dimensional as well as (usually) deeply inhomogeneous. As an example for the latter issue,
some regions of real sensorimotor spaces are often unlearnable due to inherent stochasticity or difficulty,
in which case heuristics based on the incentive to explore zones of maximal unpredictability or uncertainty,
which are often used in the field of active learning [108] [122] typically lead to catastrophic results. The issue
of high dimensionality does not only concern motor spaces, but also sensory spaces, leading to the problem
of correctly identifying, among typically thousands of quantities, those latent variables that have links to
behavioral choices. In FLOWERS, we aim at developing intrinsically motivated exploration mechanisms that
scale in those spaces, by studying suitable abstraction processes in conjunction with exploration strategies.

3.1.2. Socially Guided and Interactive Learning

Social guidance is as important as intrinsic motivation in the cognitive development of human babies [145].
There is a vast literature on learning by demonstration in robots where the actions of humans in the
environment are recognized and transferred to robots [94]. Most such approaches are completely passive: the human executes actions and the robot learns from the acquired data. Recently, the notion of interactive
learning has been introduced in [170], [101], motivated by the various mechanisms that allow humans to
socially guide a robot [158]. In an interactive context the steps of self-exploration and social guidances are not
separated and a robot learns by self exploration and by receiving extra feedback from the social context [170],
[134] [144].

Social guidance is also particularly important for learning to segment and categorize the perceptual space.
Indeed, parents interact a lot with infants, for example teaching them to recognize and name objects or
characteristics of these objects. Their role is particularly important in directing the infant attention towards
objects of interest that will make it possible to simplify at first the perceptual space by pointing out a segment
of the environment that can be isolated, named and acted upon. These interactions will then be complemented by the children own experiments on the objects chosen according to intrinsic motivation in order to improve the knowledge of the object, its physical properties and the actions that could be performed with it.

In FLOWERS, we are aiming at including intrinsic motivation system in the self-exploration part thus combining efficient self-learning with social guidance [147], [148]. We also work on developing perceptual capabilities by gradually segmenting the perceptual space and identifying objects and their characteristics through interaction with the user [34] and robots experiments [127]. Another challenge is to allow for more flexible interaction protocols with the user in terms of what type of feedback is provided and how it is provided [138]. Exploration mechanisms are combined with research in the following directions:

3.1.3. Cumulative learning, reinforcement learning and optimization of autonomous skill learning

FLOWERS develops machine learning algorithms that can allow embodied machines to acquire cumulatively sensorimotor skills. In particular, we develop optimization and reinforcement learning systems which allow robots to discover and learn dictionaries of motor primitives, and then combine them to form higher-level sensorimotor skills.

3.1.4. Autonomous perceptual and representation learning

In order to harness the complexity of perceptual and motor spaces, as well as to pave the way to higher-level cognitive skills, developmental learning requires abstraction mechanisms that can infer structural information out of sets of sensorimotor channels whose semantics is unknown, discovering for example the topology of the body or the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations towards abstract concepts and categories similar to those used by humans. Our work focuses on the study of various techniques for:

- autonomous multimodal dimensionality reduction and concept discovery;
- incremental discovery and learning of objects using vision and active exploration, as well as of auditory speech invariants;
- learning of dictionaries of motion primitives with combinatorial structures, in combination with linguistic description;
- active learning of visual descriptors useful for action (e.g. grasping);

3.1.5. Embodiment and maturational constraints

FLOWERS studies how adequate morphologies and materials (i.e. morphological computation), associated to relevant dynamical motor primitives, can importantly simplify the acquisition of apparently very complex skills such as full-body dynamic walking in biped. FLOWERS also studies maturational constraints, which are mechanisms that allow for the progressive and controlled release of new degrees of freedoms in the sensorimotor space of robots.

3.1.6. Discovering and abstracting the structure of sets of uninterpreted sensors and motors

FLOWERS studies mechanisms that allow a robot to infer structural information out of sets of sensorimotor channels whose semantics is unknown, for example the topology of the body and the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations to abstract concepts and categories similar to those used by humans.
4. Application Domains

4.1. Application Domains

**Cognitive Sciences** The computational modelling of life-long learning and development mechanisms achieved in the team centrally targets to contribute to our understanding of the processes of sensorimotor, cognitive and social development in humans. In particular, it provides a methodological basis to analyze the dynamics of the interaction across learning and inference processes, embodiment and the social environment, allowing to formalize precise hypotheses and later on test them in experimental paradigms with animals and humans. A paradigmatic example of this activity is the Neurocuriosity project achieved in collaboration with the cognitive neuroscience lab of Jacqueline Gottlieb, where theoretical models of the mechanisms of information seeking, active learning and spontaneous exploration have been developed in coordination with experimental evidence and investigation, see https://flowers.inria.fr/neurocuriosityproject/.

**Personal and lifelong learning robotics** Many indicators show that the arrival of personal robots in homes and everyday life will be a major fact of the 21st century. These robots will range from purely entertainment or educative applications to social companions that many argue will be of crucial help in our society. Yet, to realize this vision, important obstacles need to be overcome: these robots will have to evolve in unpredictable homes and learn new skills in a lifelong manner while interacting with non-engineer humans after they left factories, which is out of reach of current technology. In this context, the refoundation of intelligent systems that developmental robotics is exploring opens potentially novel horizons to solve these problems. In particular, this application domain requires advances in artificial intelligence that go beyond the current state-of-the-art in fields like deep learning. Currently these techniques require tremendous amounts of data in order to function properly, and they are severely limited in terms of incremental and transfer learning. One of our goals is to drastically reduce the amount of data required in order for this very potent field to work. We try to achieve this by making neural networks aware of their knowledge, i.e. we introduce the concept of uncertainty, and use it as part of intrinsically motivated multitask learning architectures, and combined with techniques of learning by imitation.

**Human-Robot Collaboration.** Robots play a vital role for industry and ensure the efficient and competitive production of a wide range of goods. They replace humans in many tasks which otherwise would be too difficult, too dangerous, or too expensive to perform. However, the new needs and desires of the society call for manufacturing system centered around personalized products and small series productions. Human-robot collaboration could widen the use of robot in this new situations if robots become cheaper, easier to program and safe to interact with. The most relevant systems for such applications would follow an expert worker and works with (some) autonomy, but being always under supervision of the human and acts based on its task models.

**Environment perception in intelligent vehicles.** When working in simulated traffic environments, elements of FLOWERS research can be applied to the autonomous acquisition of increasingly abstract representations of both traffic objects and traffic scenes. In particular, the object classes of vehicles and pedestrians are of interest when considering detection tasks in safety systems, as well as scene categories ("scene context") that have a strong impact on the occurrence of these object classes. As already indicated by several investigations in the field, results from present-day simulation technology can be transferred to the real world with little impact on performance. Therefore, applications of FLOWERS research that is suitably verified by real-world benchmarks has direct applicability in safety-system products for intelligent vehicles.

**Automated Tutoring Systems.** Optimal teaching and efficient teaching/learning environments can be applied to aid teaching in schools aiming both at increase the achievement levels and the reduce time needed. From a practical perspective, improved models could be saving millions of hours of students’ time (and effort) in learning. These models should also predict the achievement levels of students in order to influence teaching practices.
5. Highlights of the Year

5.1. Highlights of the Year

- P-Y. Oudeyer was invited to give the 29th Eleanor J. Gibson and James J. Gibson Lecture in Experimental Psychology, by Cornell University, US.
- P-Y. Oudeyr co-organized with colleagues at Univ. Waterloo (Canada) the interdisciplinary workshop "Designing for curiosity" at CHI 2016 in Denver, Colorado, US. This workshop aimed to build a community of academic researchers—such as computer scientists (in human-computer interaction, artificial intelligence, robotics), developmental psychologists, behavioral economists, education, marketing, neuroscience—as well as practitioners—such as painters, architects, game designers, screenwriters—who have engaged with the term curiosity in their work. Web site: https://www.crowdcurio.com/research/workshops/chi2017/.
- P-Y. Oudeyr co-organized (with V. Santucci, G. Baldassarre, A. Barto) the 3rd International Workshop on Intrinsically Motivated Open-Ended Learning (IMOL 2017). It aimed to further explore the promise of intrinsically motivated open-ended lifelong learning in robots and artificial systems. Web: http://www.imol-conf.org/. We also organized a follow-up special issue in the journal Fronties in Robotics and AI: http://goo.gl/YkMYNN.
- The Flowers team organized the 3rd "Colloque Robotique et Education" in Bordeaux (general chair: Didier Roy), gathering around 200 attendees on the topic of educational robotics. Web: http://dm1r.fr/roboeduc17/. The team also contributed to the organization of the Scratch international conference, web:http://www.scratch2017bdx.org/en/hello-world-2/.
- The Flowers team, the Potioc team and two research teams in robotics and HCI at the University of Waterloo (Canada) initiated a new interdisciplinary collaboration around the design of interactive environments that foster curiosity-driven learning, and obtained a funding from Idex/University of Bordeaux.

6. New Software andPlatforms

6.1. 3rd hand infrastructure

**KEYWORDS:** Interaction - Robotics - Infrastructure software - Framework - Robot Operating System (ROS)

**FUNCTIONAL DESCRIPTION:** The infrastructure is predicate-based to handle relational actions and covers perception (scene description generation, human actions recognition), decision making (teleoperated, scripted or learning from demonstrations), interaction with end users (GUI, voice, gestures) and parallel executions of robotic actions (hold, pick, grasp, bring, ...).

- Contact: Yoan Mollard
- URL: https://github.com/3rdHand-project/thr_infrastructure

6.2. Aversive++

**FUNCTIONAL DESCRIPTION:** Aversive++ is a C++ library that eases micro-controller programming. Its aim is to provide an interface simple enough to be able to create complex applications, and optimized enough to enable small micro-controllers to execute these applications. The other aspect of this library is to be multiplatform. Indeed, it is designed to provide the same API for a simulator (named SASIAE) and for AVR-based and ARM-based micro-controllers.

- Contact: Loïc Dauphin
- URL: http://aversiveplusplus.com/
6.3. DMP-BBO

Black-Box Optimization for Dynamic Movement Primitives

FUNCTIONAL DESCRIPTION: The DMP-BBO Matlab library is a direct consequence of the insight that black-box optimization outperforms reinforcement learning when using policies represented as Dynamic Movement Primitives. It implements several variants of the PIBB algorithm for direct policy search. The dmp-bbo C++ library has been extended to include the “unified model for regression”. The implementation of several of the function approximators have been made real-time compatible.

- Participant: Freek Stulp
- Partner: ENSTA
- Contact: Freek Stulp
- URL: https://github.com/stulp/dmpbbo

6.4. Explauto

an autonomous exploration library

SCIENTIFIC DESCRIPTION: An important challenge in developmental robotics is how robots can be intrinsically motivated to learn efficiently parametrized policies to solve parametrized multi-task reinforcement learning problems, i.e. learn the mappings between the actions and the problem they solve, or sensory effects they produce. This can be a robot learning how arm movements make physical objects move, or how movements of a virtual vocal tract modulates vocalization sounds. The way the robot will collect its own sensorimotor experience have a strong impact on learning efficiency because for most robotic systems the involved spaces are high dimensional, the mapping between them is non-linear and redundant, and there is limited time allowed for learning. If robots explore the world in an unorganized manner, e.g. randomly, learning algorithms will be often ineffective because very sparse data points will be collected. Data are precious due to the high dimensionality and the limited time, whereas data are not equally useful due to non-linearity and redundancy. This is why learning has to be guided using efficient exploration strategies, allowing the robot to actively drive its own interaction with the environment in order to gather maximally informative data to optimize the parametrized policies. In the recent year, work in developmental learning has explored various families of algorithmic principles which allow the efficient guiding of learning and exploration.

Explauto is a framework developed to study, model and simulate curiosity-driven learning and exploration in real and simulated robotic agents. Explauto’s scientific roots trace back from Intelligent Adaptive Curiosity algorithmic architecture [51], which has been extended to a more general family of autonomous exploration architectures by [3] and recently expressed as a compact and unified formalism [40]. The library is detailed in [41]. In Explauto, interest models are implementing the strategies of active selection of particular problems / goals in a parametrized multi-task reinforcement learning setup to efficiently learn parametrized policies. The agent can have different available strategies, parametrized problems, models, sources of information, or learning mechanisms (for instance imitate by mimicking vs by emulation, or asking help to one teacher or to another), and chooses between them in order to optimize learning (a processus called strategic learning [47]). Given a set of parametrized problems, a particular exploration strategy is to randomly draw goals/ RL problems to solve in the motor or problem space. More efficient strategies are based on the active choice of learning experiments that maximize learning progress using bandit algorithms, e.g. maximizing improvement of predictions or of competences to solve RL problems [51]. This automatically drives the system to explore and learn first easy skills, and then explore skills of progressively increasing complexity. Both random and learning progress strategies can act either on the motor or on the problem space, resulting in motor babbling or goal babbling strategies.

- Motor babbling consists in sampling commands in the motor space according to a given strategy (random or learning progress), predicting the expected effect, executing the command through the environment and observing the actual effect. Both the parametrized policies and interest models are finally updated according to this experience.
- Goal babbling consists in sampling goals in the problem space and to use the current policies to infer a motor action supposed to solve the problem (inverse prediction). The robot/agent then executes the command through the environment and observes the actual effect. Both the parametrized policies and interest models are finally updated according to this experience. It has been shown that this second strategy allows a progressive solving of problems much more uniformly in the problem space than with a motor babbling strategy, where the agent samples directly in the motor space [3].

![Diagram](image)

**Figure 1.** Complex parametrized policies involve high dimensional action and effect spaces. For the sake of visualization, the motor M and sensory S spaces are only 2D each in this example. The relationship between M and S is non-linear, dividing the sensorimotor space into regions of unequal stability: small regions of S can be reached very precisely by large regions of M, or large regions in S can be very sensitive to variations in M; s as well as a non-linear and redundant relationship. This non-linearity can imply redundancy, where the same sensory effect can be attained using distinct regions in M.

**FUNCTIONAL DESCRIPTION:** This library provides high-level API for an easy definition of:
- Real and simulated robotic setups (Environment level),
- Incremental learning of parametrized policies (Sensorimotor level),
- Active selection of parametrized RL problems (Interest level).

The library comes with several built-in environments. Two of them corresponds to simulated environments: a multi-DoF arm acting on a 2D plan, and an under-actuated torque-controlled pendulum. The third one allows to control real robots based on Dynamixel actuators using the Pypot library. Learning parametrized policies involves machine learning algorithms, which are typically regression algorithms to learn forward models, from motor controllers to sensory effects, and optimization algorithms to learn inverse models, from sensory effects, or problems, to the motor programs allowing to reach them. We call these sensorimotor learning algorithms sensorimotor models. The library comes with several built-in sensorimotor models: simple nearest-neighbor look-up, non-parametric models combining classical regressions and optimization algorithms, online mixtures of Gaussians, and discrete Lidstone distributions. Explauto sensorimotor models are online learning algorithms, i.e. they are trained iteratively during the interaction of the robot in the environment in which it evolves. Explauto provides also a unified interface to define exploration strategies using the InterestModel class. The library comes with two built-in interest models: random sampling as well as sampling maximizing the learning progress in forward or inverse predictions.

Explauto environments now handle actions depending on a current context, as for instance in an environment where a robotic arm is trying to catch a ball: the arm trajectories will depend on the current position of the ball (context). Also, if the dynamic of the environment is changing over time, a new sensorimotor model
(Non-Stationary Nearest Neighbor) is able to cope with those changes by taking more into account recent experiences. Those new features are explained in Jupyter notebooks.

This library has been used in many experiments including:

- the control of a 2D simulated arm,
- the exploration of the inverse kinematics of a poppy humanoid (both on the real robot and on the simulated version),
- acoustic model of a vocal tract.

Explauto is crossed-platform and has been tested on Linux, Windows and Mac OS. It has been released under the GPLv3 license.

- Contact: Sébastien Forestier
- URL: https://github.com/flowersteam/explauto

6.5. HiPi Board

**FUNCTIONAL DESCRIPTION:** HiPi is a board to control robots on Raspberry Pi. It is an extension of the Pixl board with the following features:

- A DC/DC power converter from 12V (motor) to 5V (Raspberry Pi) at 3A.
- A stereo audio amplifier 3W.
- A MPU9250 central motion unit.
- A RS232 and a RS485 bus connected to the Raspberry Pi by SPI for driving MX and RX Dynamixel motor series.

This board will be integrated soon in the new head of the Poppy Humanoid and Poppy Torso.

Using the Raspberry Pi for every Poppy robots will simplify the hardware complexity (we maintain 4 types of embedded boards, with different Linux kernel and configurations) and improve the usage and installation of new robots.

- Contact: Theo Segonds
- URL: https://forum.poppy-project.org/t/poppy-1-1-hipi/2137

6.6. IKPy

**Inverse Kinematics Python Library**

**FUNCTIONAL DESCRIPTION:** IKPy is a Python Inverse Kinematics library, designed to be simple to use and extend. It provides Forward and Inverse kinematics functionality, bundled with helper tools such as 3D plotting of the kinematics chains. Being written entirely in Python, IKPy is lightweight and is based on numpy and scipy for fast optimization. IKPy is compatible with many robots, by automatically parsing URDF files. It also supports other (such as DH-parameters) and custom representations. Moreover, it provides a framework to easily implement new Inverse Kinematics strategies. Originally developed for the Poppy project, it can also be used as a standalone library.

- Contact: Pierre Manceron
- URL: https://github.com/Phylliade/ikpy

6.7. KERAS-QR

**KERAS with Quick Reset**

**KEYWORDS:** Library - Deep learning

- Participant: Florian Golemo
- Contact: Florian Golemo
- URL: https://github.com/fgolemo/keras
6.8. KidBreath

**FUNCTIONAL DESCRIPTION:** KidBreath is a web responsive application composed by several interactive contents linked to asthma and displayed to different forms: learning activities with quiz, short games and videos. There are profile creation and personalization, and a part which describes historic and scoring of learning activities, to see evolution of KidBreath use. To test Kidlearn algorithm, it is adapted and integrated on this platform. Development in PHP, HTML-5, CSS, MySQL, JQuery, Javascript. Hosting in APACHE, LINUX, PHP 5.5, MySQL, OVH.

- Partner: ItWell SAS
- Contact: Alexandra Delmas
- URL: http://www.kidbreath.fr

6.9. Kidlearn: money game application

**FUNCTIONAL DESCRIPTION:** The games are instantiated in a browser environment where students are proposed exercises in the form of money/token games (see Figure 2). For an exercise type, one object is presented with a given tagged price and the learner has to choose which combination of bank notes, coins or abstract tokens need to be taken from the wallet to buy the object, with various constraints depending on exercises parameters. The games have been developed using web technologies, HTML5, javascript and Django.

![Figure 2. Four principal regions are defined in the graphical interface. The first is the wallet location where users can pick and drag the money items and drop them on the repository location to compose the correct price. The object and the price are present in the object location. Four different types of exercises exist: M: customer/one object, R: merchant/one object, MM: customer/two objects, RM: merchant/two objects.](image)

- Contact: Benjamin Clement
- URL: https://flowers.inria.fr/research/kidlearn/

6.10. Kidlearn: script for Kidbreath use

**FUNCTIONAL DESCRIPTION:** A new way to test Kidlearn algorithms is to use them on Kidbreath Platform. The Kidbreath Platform use apache/PHP server, so to facilitate the integration of our algorithm, a python script have been made to allow PHP code to use easily the python library already made which include our algorithms.

Github link to explanation about it: https://github.com/flowersteam/kidlearn/

- Contact: Benjamin Clement
6.11. KidLearn

**KEYWORD:** Automatic Learning

**FUNCTIONAL DESCRIPTION:** KidLearn is a software which adaptively personalize sequences of learning activities to the particularities of each individual student. It aims at proposing to the student the right activity at the right time, maximizing concurrently his learning progress and its motivation.

- Participants: Benjamin Clement, Didier Roy, Manuel Lopes and Pierre Yves Oudeyer
- Contact: Manuel Lopes
- URL: https://flowers.inria.fr/research/kidlearn/

6.12. Kinect 2 Server

**Kinect 2 server**

**KEYWORDS:** Depth Perception - Speech recognition - Gesture recognition - Kinect

**FUNCTIONAL DESCRIPTION:** The server written in C# uses the Kinect SDK v2 to get the RGBD raw image, skeleton tracking information, recognized speech. It also uses the text-to-speech from Microsoft. Then it streams JSON data over the network using the Publisher/Subscriber pattern from the ZeroMQ network library. A Linux client has been written in Python but it can be written in any other language that is compatible with ZeroMQ. Features are controllable through a Graphical User Interface on Windows, or through the code from any Linux/Windows client. The clients can for instance enable features (speech recognition on, skeleton tracking off, . . . ) and parameters (set new speech to recognize, change language, . . . ) from remote.

- Contact: Yoan Mollard
- URL: https://github.com/baxter-flowers/kinect_2_server/

6.13. Multimodal

**FUNCTIONAL DESCRIPTION:** The python code provides a minimum set of tools and associated libraries to reproduce the experiments in [98] , together with the choreography datasets. The code is primarily intended for reproduction of the multimodal learning experiment mentioned above. It has already been reused in several experimentations by other member of the team and is expected to play an important role in further collaborations. It is also expected that the public availability of the code encourages further experimentation by other scientists with data coming from other domains, thus increasing both the impact of the aforementioned publication and the knowledge on the algorithm behaviors.

- Participant: Olivier Mangin
- Contact: Olivier Mangin
- URL: https://github.com/omangin/multimodal

6.14. OptiTrack

**FUNCTIONAL DESCRIPTION:** This python library allows you to connect to an OptiTrack from NaturalPoint. This camera permits the tracking of 3D markers efficiently and robustly. With this library, you can connect to the Motive software used by the OptiTrack and retrieve the 3D position and orientation of all your tracked markers directly from python.

- Participant: Pierre Rouanet
- Contact: Pierre Rouanet
- URL: http://www.optitrack.com/
6.15. Pixl Board

**FUNCTIONAL DESCRIPTION:** Pixl is a tiny board used to create low cost robots based on Raspberry Pi board and Dynamixel XL-320 motors. This board has 2 main features:

- The power part, allowing the user to plug a 7.5V AC/DC converter or a battery directly into the Pixl. This power is distributed to all XL320 motors and is converted to 5V for the Raspberry Pi board.
- The communication part, which converts full duplex to half duplex and vice-versa. The half duplex part switch between RX and TX automatically. Another connector allows the user to connect his XL320 network.

The board is used in the Poppy Ergo Jr robot.

- Contact: Theo Segonds
- URL: [https://github.com/poppy-project/pixl](https://github.com/poppy-project/pixl)

6.16. Poppy

**FUNCTIONAL DESCRIPTION:** The Poppy Project team develops open-source 3D printed robots platforms based on robust, flexible, easy-to-use and reproduce hardware and software. In particular, the use of 3D printing and rapid prototyping technologies is a central aspect of this project, and makes it easy and fast not only to reproduce the platform, but also to explore morphological variants. Poppy targets three domains of use: science, education and art.

In the Poppy project we are working on the Poppy System which is a new modular and open-source robotic architecture. It is designed to help people create and build custom robots. It permits, in a similar approach as Lego, building robots or smart objects using standardized elements.

Poppy System is a unified system in which essential robotic components (actuators, sensors...) are independent modules connected with other modules through standardized interfaces:

- Unified mechanical interfaces, simplifying the assembly process and the design of 3D Printable parts.
- Unified communication between elements using the same connector and bus for each module.
- Unified software, making it easy to program each module independently.

Our ambition is to create an ecosystem around this system so communities can develop custom modules, following the Poppy System standards, which can be compatible with all other Poppy robots.

- Participants: Jonathan Grizou, Matthieu Lapeyre, Pierre Rouanet and Pierre-Yves Oudeyer
- Contact: Pierre-Yves Oudeyer
- URL: [https://www.poppy-project.org/](https://www.poppy-project.org/)

6.17. Poppy Ergo Jr

**FUNCTIONAL DESCRIPTION:** Poppy Ergo Jr is an open hardware robot developed by the Poppy Project to explore the use of robots in classrooms for learning robotic and computer science.

It is available as a 6 or 4 degrees of freedom arm designed to be both expressive and low-cost. This is achieved by the use of FDM 3D printing and low cost Robotis XL-320 actuators. A Raspberry Pi camera is attached to the robot so it can detect object, faces or QR codes.

The Ergo Jr is controlled by the Pypot library and runs on a Raspberry pi 2 or 3 board. Communication between the Raspberry Pi and the actuators is made possible by the Pixl board we have designed.

The Poppy Ergo Jr robot has several 3D printed tools extending its capabilities. There are currently the lampshade, the gripper and a pen holder.
Figure 3. Poppy Ergo Jr, 6-DoFs arm robot for education

Figure 4. The available Ergo Jr tools: a pen holder, a lampshade and a gripper
With the release of a new Raspberry Pi board early 2016, the Poppy Ergo Jr disk image was updated to support Raspberry Pi 2 and 3 boards. The disk image can be used seamlessly with a board or the other.

- Contact: Theo Segonds
- URL: https://github.com/poppy-project/poppy-ergo-jr

### 6.18. Poppy Ergo Jr Installer

**FUNCTIONAL DESCRIPTION:** An alternative way to install the Ergo Jr robot software is made available using containers.

Users can own their own operating system installation, then add the Ergo Jr required software in a sandboxed environment. This results in a non-intrusive installation on the host system.

Docker containers implementation were used, and image is hosted at Docker Hub.

- Contact: Damien Caselli
- URL: https://hub.docker.com/r/poppycommunity/ergo-jr/

### 6.19. Poppy Ergo Jr Simulator

**FUNCTIONAL DESCRIPTION:** Poppy Project, through Poppy Education, wants users to get used to robotics, even without owning a physical robot.

For that purpose, Poppy Project team created a dummy robot in Pypot that is meant to be used in conjunction with a consumer application. We choose to develop a web hosted application using a 3D engine (Threejs) to render the robot.

Our ambition is to have a completely standalone simulated robot with physics. Some prototypes were created to benchmark possible solutions.

- Contact: Damien Caselli
- URL: https://github.com/poppy-project/poppy-simu

### 6.20. ProMP

**Probabilistic Movement Primitives**

**KEYWORDS:** Interaction - Robotics - Probability - Motion model - Robot Operating System (ROS)

**FUNCTIONAL DESCRIPTION:** Joint-space primitives with a task-space constraint: The primitives are stored in joint-space but demonstrations are provided both in joint space and task space, context. Thanks to this context, task-space goals can be requested to these joint-space primitives. The benefit is that requesting a new task-space goal does not require to call an IK method which would return demonstrations-agnostic joint configurations.

Vocal interactive learning and clustering: This work includes an interactive learning aspect which allows to automatically cluster motor primitives based on the standard deviation of their demonstrations. A new primitive is created automatically if the provided demonstration is out of 2 standard deviation of the existing primitives, otherwise the demonstration is distributed to an existing one.

- Contact: Yoan Mollard
- URL: https://github.com/baxter-flowers/promplib

### 6.21. PyPot

**SCIENTIFIC DESCRIPTION:** PyPot is a framework developed to make it easy and fast to control custom robots based on Dynamixel motors. This framework provides different levels of abstraction corresponding to different types of use. PyPot can be used to:

- control Robotis motors through a USB2serial device,
- define the structure of a custom robot and control it through high-level commands,
- define primitives and easily combine them to create complex behavior.
Pypot is part of the Poppy project. It is the core library used by the Poppy robots. This abstraction layer allows to seamlessly switch from a given Poppy robot to another. It also provides a common set of tools, such as forward and inverse kinematics, simple computer vision, recording and replaying moves, or easy access to the autonomous exploration library Explauto.

To extend pypot application domains and connection to outside world, it also provides an HTTP API. On top of providing an easy way to connect to smart sensors or connected devices, it is notably used to connect to Snap!, a variant of the well-known Scratch visual programming language.

**Figure 5. Example of using pypot to program a robot to reproduce a drawn shape**

**FUNCTIONAL DESCRIPTION:** Pypot is entirely written in Python to allow for fast development, easy deployment and quick scripting by non-expert developers. It can also benefit from the scientific and machine learning libraries existing in Python. The serial communication is handled through the standard library and offers high performance (10ms sensorimotor loop) for common Poppy uses. It is cross-platform and has been tested on Linux, Windows and Mac OS.

Pypot is also compatible with the V-REP simulator. This allows the transparent switch from a real robot to its simulated equivalent with a single code base.

Finally, it has been developed to be easily and quickly extended for other types of motors and sensors.

It works with Python 2.7 or Python 3.3 or later, and has also been adapted to the Raspberry Pi board.

Pypot has been connected to Snap!, a variant of the famous Scratch visual language, developed to teach computer science to children. It is based on a drag-and-drop blocks interface to write scripts by assembling those blocks.

Thanks to the Snap! HTTP block, a connection can be made to pypot allowing users to directly control robots through their visual interfaces. A set of dedicated Snap! blocks have been designed, such as *set motor position* or *get motor temperature*. Thanks to the Snap! HTTP block, users can control robots through this visual interfaces connecting to Pypot. A set of dedicated Snap! blocks has been designed, such as *set motor position* or *get motor temperature*.

Snap! is also used as a tool to program the robot by demonstration. Using the *record* and *play* blocks, users can easily trigger kinesthetic recording of the whole robot or only a specific subpart, such as an arm. These records can then be played or ‘mixed’ - either played in sequence or simultaneously - with other recordings to compose complex choreographies. The moves are encoded as a model of mixture of gaussians (GMM) which allows the definition of clean mathematical operators for combining them.

This recording tool has been developed and used in collaboration with artists who show interest in the concept of robotic moves.
Figure 6. Using Snap! to program a robot by demonstration and create complex choreographies

Figure 7. Artistic project exploring the concept of robotic move.
• Participants: Damien Caselli, Matthieu Lapeyre, Pierre Rouanet, Steve Nguyen and Theo Segonds
• Contact: Theo Segonds
• URL: https://github.com/poppy-project/pypot

6.22. PyQMC

*FUNCTIONAL DESCRIPTION:* PyQMC is a python library implementing the control method described in http://dx.doi.org/10.1371/journal.pone.0083411 It allows to solve discrete markovian decision processes by computing a Quasi-Metric on the state space. This model based method has the advantage to be goal independent and thus can produce a policy for any goal with relatively few recomputation. New addition to this method is the possibility of online learning of the transition model and the Quasi-Metric.

• Participant: Steve Nguyen
• Contact: Steve Nguyen
• URL: https://github.com/SteveNguyen/pyqmc

6.23. ROS Optitrack Publisher

*KEYWORDS:* Target tracking - Robot Operating System (ROS)

*FUNCTIONAL DESCRIPTION:* This package allows to publish optitrack markers declared as rigid bodies as TF transforms. Data is gathered through the embedded VRPN server of Motive/Arena. Only rigid bodies are requested to the server, thus single points in 2D/3D are ignored. VRPN server can be enable in View > Data streaming in Motive.

• Contact: Yoan Mollard
• URL: https://github.com/baxter-flowers/optitrack_publisher

6.24. ThifloNet

*KEYWORDS:* Deep learning - Policy Learning

*SCIENTIFIC DESCRIPTION:* We created a software architecture that combines a state-of-the-art computer vision system with a policy learning framework. This system is able to perceive a visual scene, given by a still image, extract facts (“predicates”), and propose an optimal action to achieve a given goal. Both systems are chained into a pipeline that is trained by presenting images and demonstrating an optimal action. By providing this information, both the predicate recognition model and the policy learning model are updated.

Our architecture is based on the recent works of Lerer, A., Gross, S., & Fergus, R., 2016 (“Learning Physical Intuition of Block Towers by Example”). They created a large network able to identify physical properties of stacked blocks. Analogously our vision system utilizes the same network layout (without the image prediction auxiliary output), with an added output layer for predicates, based on the expected number and arity of predicates. The vision subsystem is not trained with a common cross-entropy or MSE loss function, but instead receives its loss form the policy learning subsystem. The policy learning module calculates the loss as optimal combination of predicates for the given expert action.

By using this combination of systems, the architecture as a whole requires significantly fewer data samples than other systems (which exclusively utilize neural networks). This makes the approach more feasible to real-life application with actual live demonstration.

*FUNCTIONAL DESCRIPTION:* The neural network consists of ResNet-50 (the currently best-performing computer vision system), with 50 layers, 2 layers for converting the output of ResNet to predicates and a varying amount of output neurons, corresponding to the estimated number of n-arity predicates. The network was pretrained on the ImageNet dataset. The policy learning module incorporates the ACE tree learning tool and a wrapper in Prolog.
Our example domain consists of 2-4 cubes colored in red, blue, green, and yellow and randomly stacked on top of each other in a virtual 3D environment. The dataset used for training and testing contains a total of 30000 elements, each with an image of the scene, the correct predicates, a list of blocks that are present and the corresponding expert action, that would lead to stacking the blocks to a tower.

- Participants: Florian Golemo, Manuel Lopes and Thibaut Munzer
- Contact: Florian Golemo

7. New Results

7.1. Computational Models Of Human Development and Cognition

7.1.1. Computational Models Of Information-Seeking and Curiosity-Driven Learning in Humans and Animals

Participants: Pierre-Yves Oudeyer [correspondant], William Schueller, Sebastien Forestier, Alvaro Ovalle.

This project involves a collaboration between the Flowers team, the Cognitive Neuroscience Lab of J. Gottlieb at Columbia Univ. (NY, US), and the developmental psychology lab of Celeste Kidd at Univ. Rochester, US, on the understanding and modeling of mechanisms of curiosity, attention and active intrinsically motivated exploration that until now have been little explored in neuroscience, machine learning and cognitive robotics. It is organized around the study of the hypothesis that information gain (or control gain) could generate intrinsic reward in the brain (living or artificial), driving attention and exploration independently from material rewards, and allowing for autonomous lifelong acquisition of open repertoires of skills. The project combines expertise about attention and exploration in the brain and a strong methodological framework for conducting experimentations with monkeys, human adults (Gottlieb’s lab) and children (Kidd’s lab) together with computational modeling of curiosity/intrinsic motivation and learning in the Flowers team.

Such a collaboration paves the way towards a central objective, which is now a central strategic objective of the Flowers team: designing and conducting experiments in animals and humans informed by computational/mathematical theories of information seeking, and allowing to test the predictions of these computational theories.

7.1.1.1. Context

Curiosity can be understood as a family of mechanisms that evolved to allow agents to maximize their knowledge (or their control) of the useful properties of the world - i.e., the regularities that exist in the world - using active, targeted investigations. In other words, we view curiosity as a decision process that maximizes learning/competence progress (rather than minimizing uncertainty) and assigns value (“interest”) to competing tasks based on their epistemic qualities - i.e., their estimated potential allow discovery and learning about the structure of the world.

Because a curiosity-based system acts in conditions of extreme uncertainty (when the distributions of events may be entirely unknown) there is in general no optimal solution to the question of which exploratory action to take [31], [152], [160]. Therefore we hypothesize that, rather than using a single optimization process as it has been the case in most previous theoretical work [120], curiosity is comprised of a family of mechanisms that include simple heuristics related to novelty/surprise and measures of learning progress over longer time scales [150] [98], [146]. These different components are related to the subject’s epistemic state (knowledge and beliefs) and may be integrated with fluctuating weights that vary according to the task context. We will quantitatively characterize this dynamic, multi-dimensional system in the framework of Bayesian Reinforcement Learning, as described below.
Because of its reliance on epistemic currencies, curiosity is also very likely to be sensitive to individual differences in personality and cognitive functions. Humans show well-documented individual differences in curiosity and exploratory drives [137], [159], and rats show individual variation in learning styles and novelty seeking behaviors [115], but the basis of these differences is not understood. We postulate that an important component of this variation is related to differences in working memory capacity and executive control which, by affecting the encoding and retention of information, will impact the individual’s assessment of learning, novelty and surprise and ultimately, the value they place on these factors [156], [168], [93], [174]. To start understanding these relationships, about which nothing is known, we will search for correlations between curiosity and measures of working memory and executive control in the population of children we test in our tasks, analyzed from the point of view of a computational model based on Bayesian reinforcement learning.

A final premise guiding our research is that essential elements of curiosity are shared by humans and non-human primates. Human beings have a superior capacity for abstract reasoning and building causal models, which is a prerequisite for sophisticated forms of curiosity such as scientific research. However, if the task is adequately simplified, essential elements of curiosity are also found in monkeys [137], [132] and, with adequate characterization, this species can become a useful model system for understanding the neurophysiological mechanisms.

7.1.1.2. Objectives

Our studies have several highly innovative aspects, both with respect to curiosity and to the traditional research field of each member team.

- Linking curiosity with quantitative theories of learning and decision making: While existing investigations examined curiosity in qualitative, descriptive terms, here we propose a novel approach that integrates quantitative behavioral and neuronal measures with computationally defined theories of Bayesian Reinforcement Learning and decision making.

- Linking curiosity in children and monkeys: While existing investigations examined curiosity in humans, here we propose a novel line of research that coordinates its study in humans and non-human primates. This will address key open questions about differences in curiosity between species, and allow access to its cellular mechanisms.

- Neurophysiology of intrinsic motivation: Whereas virtually all the animal studies of learning and decision making focus on operant tasks (where behavior is shaped by experimenter-determined primary rewards) our studies are among the very first to examine behaviors that are intrinsically motivated by the animals’ own learning, beliefs or expectations.

- Neurophysiology of learning and attention: While multiple experiments have explored the single-neuron basis of visual attention in monkeys, all of these studies focused on vision and eye movement control. Our studies are the first to examine the links between attention and learning, which are recognized in psychophysical studies but have been neglected in physiological investigations.

- Computer science: biological basis for artificial exploration: While computer science has proposed and tested many algorithms that can guide intrinsically motivated exploration, our studies are the first to test the biological plausibility of these algorithms.

- Developmental psychology: linking curiosity with development: While it has long been appreciated that children learn selectively from some sources but not others, there has been no systematic investigation of the factors that engender curiosity, or how they depend on cognitive traits.

7.1.1.3. Current results

In particular, new works and results in 2017 include:

7.1.1.4. Experiments in Active Categorization

In 2017, we have been occupied by the implementation, running and analysis of the human adult experiment piloted the year before. A distinguishing feature of curiosity is that, rather than seeking to obtain information in a known task context (e.g., reading the menu in a restaurant) curiosity has to discover regularities whose existence is a priori unknown. This raises the question of how active learners become interested in specific
items: how do agents decide which task to be interested in – i.e., allocate “study time” - given that the underlying rewards or patterns are sparse and unknown? A theoretical solution to this problem is suggested by the optimal learning literature, and proposes that allocation of resources may be based on the relative difficulty of competing tasks, or the learning progress (LP) expected from engaging a task. While these strategies can make equivalent predictions in certain simple situations (e.g., when learning curves are known and concave), LP-based mechanisms are superior in open-ended environments that contain unlearnable tasks. In such situations, LP-based strategies assign lower value to tasks where little progress is made and allow the learner to disengage from such tasks, while performance-based mechanisms, by assigning higher value to the lower-competence task, can push the learner to labor in vain. In the present experiment we asked whether humans possess, and use, metacognitive abilities to guide performance-based or LP-based exploration in two contexts in which they could freely choose to learn about 4 competing tasks. Participants (n = 505, recruited via Amazon Mechanical Turk) were tested on a paradigm in which they could freely choose to engage with one of four different classification tasks. We are currently analyzing the results and working on a computational models of the underlying cognitive and motivational mechanisms.

7.1.2. Computational Models Of Tool Use and Speech Development: the Roles of Active Learning, Curiosity and Self-Organization

Participants: Pierre-Yves Oudeyer [correspondant], Sébastien Forestier.

7.1.2.1. Modeling Speech and Tool Use Development in Infants

A scientific challenge in developmental and social robotics is to model how autonomous organisms can develop and learn open repertoires of skills in high-dimensional sensorimotor spaces, given limited resources of time and energy. This challenge is important both from the fundamental and application perspectives. First, recent work in robotic modeling of development has shown that it could make decisive contributions to improve our understanding of development in human children, within cognitive sciences [120]. Second, these models are key for enabling future robots to learn new skills through lifelong natural interaction with human users, for example in assistive robotics [154].

In recent years, two strands of work have shown significant advances in the scientific community. On the one hand, algorithmic models of active learning and imitation learning combined with adequately designed properties of robotic bodies have allowed robots to learn how to control an initially unknown high-dimensional body (for example locomotion with a soft material body [3]). On the other hand, other algorithmic models have shown how several social learning mechanisms could allow robots to acquire elements of speech and language [105], allowing them to interact with humans. Yet, these two strands of models have so far mostly remained disconnected, where models of sensorimotor learning were too “low-level” to reach capabilities for language, and models of language acquisition assumed strong language specific machinery limiting their flexibility. Preliminary work has been showing that strong connections are underlying mechanisms of hierarchical sensorimotor learning, artificial curiosity, and language acquisition [54].

Recent robotic modeling work in this direction has shown how mechanisms of active curiosity-driven learning could progressively self-organize developmental stages of increasing complexity in vocal skills sharing many properties with the vocal development of infants [39]. Interestingly, these mechanisms were shown to be exactly the same as those that can allow a robot to discover other parts of its body, and how to interact with external physical objects [149].

In such current models, the vocal agents do not associate sounds to meaning, and do not link vocal production to other forms of action. In other models of language acquisition, one assumes that vocal production is mastered, and hand code the meta-knowledge that sounds should be associated to referents or actions [105]. But understanding what kind of algorithmic mechanisms can explain the smooth transition between the learning of vocal sound production and their use as tools to affect the world is still largely an open question.

The goal of this work is to elaborate and study computational models of curiosity-driven learning that allow flexible learning of skill hierarchies, in particular for learning how to use tools and how to engage in social interaction, following those presented in [51], [3], [45], [39]. The aim is to make steps towards addressing the
fundamental question of how speech communication is acquired through embodied interaction, and how it is linked to tool discovery and learning.

We take two approaches to study those questions. One approach is to develop robotic models of infant development by looking at the developmental psychology literature about tool use and speech and trying to implement and test the psychologists’ hypotheses about the learning mechanisms underlying infant development. Our second approach is to directly collaborate with developmental psychologists to analyze together the data of their experiments and develop other experimental setup that are well suited to answering modeling questions about the underlying exploration and learning mechanisms. We thus started to collaborate with Lauriane Rat-Fischer, a developmental psychologist working in Toulouse on the emergence of tool use in the first years of human life. We are currently analyzing together the behaviour of 22 month old infants in a tool use task where the infants have to retrieve a toy put in the middle of a tube by inserting sticks into the tube and pushing the toy out. We are looking at the different actions of the infant with tools and toys but also its looking behaviour, towards the tool, toys or the experimenter, and we are trying to infer the goals and exploration strategies of the infant.

In our recent robotic modeling work, we showed that the Model Babbling learning architecture allows the development of tool use in a robotic setup, through several fundamental ideas. First, goal babbling is a powerful form of exploration to produce a diversity of effects by self-generating goals in a task space. Second, the possible movements of each object define a task space in which to choose goals, and the different task spaces form an object-based representation that facilitates prediction and generalization. Also, cross-learning between tasks updates all skills while exploring one in particular. A novel insight was that early development of tool use could happen without a combinatorial action planning mechanism: modular goal babbling in itself allowed the emergence of nested tool use behaviors.

This year we extended this architecture so that the agent can imitate caregiver’s sounds in addition to exploring autonomously [78]. We hypothesized that these same algorithmic ingredients could allow a joint unified development of speech and tool use. Our learning agent is situated in a simulated environment where a vocal tract and a robotic arm are to be explored with the help of a caregiver. The environment is composed of three toys, one stick that can be used as a tool to move toys, and a caregiver moving around. The caregiver helps in two ways. If the agent touches a toy, the caregiver produces this toy’s name, but otherwise produces a distractor word as if it was talking to another adult. If the agent produces a sound close to a toy’s name, the caregiver moves this toy within agent reach 8.

We show that our learning architecture based on Model Babbling allows agents to learn how to 1) use the robotic arm to grab a toy or a stick, 2) use the stick as a tool to get a toy, 3) learn to produce toy names with the vocal tract, 4) use these vocal skills to get the caregiver to bring a specific toy within reach, and 5) choose the most relevant of those strategies to retrieve a toy that can be out-of-reach. Also, the grounded exploration of toys accelerates the learning of the production of accurate sounds for toy names once the caregiver is able to recognize them and react by bringing them within reach, with respect to distractor sounds without any meaning in the environment. Our model is the first to allow the study of the early development of tool use and speech in a unified framework.

This model focuses on the role of one important form of body babbling where exploration is directed towards self-generated goals in free play, combined with imitation learning of a contingent caregiver. This model does not assume capabilities for complex sequencing and combinatorial planning which are often considered necessary for tool use. Yet, we show that the mechanisms in this model allow a learner to progressively discover how to grab objects with the hand, how to use objects as tools to reach further objects, how to produce vocal sounds, and how to leverage these vocal sounds to use a caregiver as a social tool to retrieve objects. Also, the discovery that certain sounds can be used as a social tool further guides vocal learning. This model predicts that infants learn to vocalize the name of toys in a natural play scenario faster than learning other words because they often choose goals related to those toys and engage caregiver’s help by trying to vocalize those toys’ names. We presented those results at the 39th Annual Conference of the Cognitive Science Society (CogSci 2017).
7.1.3. Computational Models Of Developmental Exploration Mechanisms in Vocal Babbling and Arm Reaching in Infants

Participants: Pierre-Yves Oudeyer [correspondent], Clement Moulin-Frier, Freek Stulp, Jules Brochard.

7.1.3.1. Proximodistal Exploration in Motor Learning as an Emergent Property of Optimization

To harness the complexity of their high-dimensional bodies during sensorimotor development, infants are guided by patterns of freezing and freeing of degrees of freedom. For instance, when learning to reach, infants free the degrees of freedom in their arm proximodistally, i.e. from joints that are closer to the body to those that are more distant. We formulated and studied computationally the hypothesis that such patterns can emerge spontaneously as the result of a family of stochastic optimization processes (evolution strategies with covariance-matrix adaptation), without an innate encoding of a maturational schedule. In particular, we made simulated experiments with an arm where a computational learner progressively acquires reaching skills through adaptive exploration, and we showed that a proximodistal organization appears spontaneously, which we denoted PDFF (ProximoDistal Freezing and Freeing of degrees of freedom). We also compared this emergent organization between different arm morphologies – from human-like to quite unnatural ones – to study the effect of different kinematic structures on the emergence of PDFF. This work was published in the journal Developmental Science[74].

7.1.3.2. Emergent Jaw Predominance in Vocal Development through Stochastic Optimization

Infant vocal babbling is strongly relying on jaw oscillations, especially at the stage of canonical babbling, which underlies the syllabic structure of world languages. We have proposed, modelled and analyzed an hypothesis to explain this predominance of the jaw in early babbling. This hypothesis states that general stochastic optimization principles, when applied to learning sensorimotor control, automatically generate ordered babbling stages with a predominant exploration of jaw movements in early stages, just like they generate proximo-distal organization of exploration in arm reaching as described in the paragraph above. In particular, such stochastic optimization principles predominantly explore jaw movement at the beginning of vocal learning, and when close to the rest position of the vocal tract, as it impacts the auditory effects more than
other articulators. This work was published in the journal *IEEE Transactions on Cognitive and Developmental Systems* [73].

### 7.1.4. Models of Self-organization of lexical conventions: the role of Active Learning and Active Teaching in Naming Games

**Participants:** William Schueller [correspondent], Pierre-Yves Oudeyer.

How does language emerge, evolve and gets transmitted between individuals? What mechanisms underly the formation and evolution of linguistic conventions, and what are their dynamics? Computational linguistic studies have shown that local interactions within groups of individuals (e.g. humans or robots) can lead to self-organization of lexica associating semantic categories to words [165]. However, it still doesn’t scale well to complex meaning spaces and a large number of possible word-meaning associations (or lexical conventions), suggesting high competition among those conventions.

In statistical machine learning and in developmental sciences, it has been argued that an active control of the complexity of learning situations can have a significant impact on the global dynamics of the learning process [120] [130] [139]. This approach has been mostly studied for single robotic agents learning sensorimotor affordances [150][40]. However active learning might represent an evolutionary advantage for language formation at the population level as well [54] [167].

Naming Games are a computational framework, elaborated to simulate the self-organization of lexical conventions in the form of a multi-agent model [166]. Through repeated local interactions between random couples of agents (designated speaker and hearer), shared conventions emerge. Interactions consist of uttering a word – or an abstract signal – referring to a topic, and evaluating the success or failure of communication.

However, in existing works processes involved in these interactions are typically random choices, especially the choice of a communication topic.

The introduction of active learning algorithms in these models produces significant improvement of the convergence process towards a shared vocabulary, with the speaker [49], [60] [109] or the hearer [61] actively controlling vocabulary growth.

#### 7.1.4.1. Definition of a local measure of convergence for the Naming Game: Local Approximated Probability of Success (LAPS), using limited memory of past interactions

In the Naming Game, one measure is usually used to represent the state of convergence of the population: the success rate, or probability of success at a given time step. It increases over time, from 0 to 1. This measure is however global, and not accessible to individual agents; in which case it would have been a perfect candidate for a functional whose maximization would drive local behavior. Several other measures have been suggested, as one based on local information gain, or entropy reduction [60]. Those measures however are either defined in a very constrained case (without synonymy and homonymy, and fixed and known numbers of words and meanings), and their minimization can actually block the process of convergence – as their evolution is not easily predictable.

Instead, we defined a local approximation of the success rate. For this, we need a representation of the state of the population. This is done by constructing an average vocabulary representing the population, using a partial memory of the past interactions. This vocabulary is then used together with the agent’s own vocabulary to compute a probability of success. A key element of this measure is the time scale associated to the memory: in fact, it allows not only to define a degree of certainty of a given association, but also a degree of uncertainty at a higher level (word or meaning). This measure is local (available to an agent through only its own knowledge) but its convergence to 100% is bound to global dynamics. In other words, we can use it as a functional to maximize at the local level to reinforce agreement at the population level.

#### 7.1.4.2. Active Topic Choice: LAPS and Multi-Armed Bandits

Usually, the topic used in an interaction of the Naming Game is picked randomly. A first way of introducing active control of complexity growth is through the mechanism of topic choice: choosing it according to past memory. It allows each agent to balance reinforcement of known associations and invention of new ones,
which can be seen as an exploitation vs. exploration problem. This can speed up convergence processes, and even lower significantly local and global complexity: for example in [60], [61], where heuristics based on the number of past successful interactions were used.

However, we can now define new strategies directly maximizing the LAPS measure. At each step, the agent picking a topic will choose one that yields maximum expected increase of the LAPS measure. However, this expected value being computationally really costly, we use a Multi-Armed Bandit algorithm. At the beginning, only one machine is available, the exploration machine. When used by the agent, its parameters are updated through Thompson Sampling algorithm, and a new machine is created with the exact same parameters, corresponding to the newly explored meaning. At any time, the number of machines available to the agent is then equal to the number of already known meanings, plus one (the exploration machine).

This strategy can speed up convergence the convergence process, but also diminishes significantly the global complexity – i.e. the maximum number of distinct word-meaning association present in the population. See figure 10.

7.1.4.3. Acceptance policy: Updating or not vocabulary based on memory of past interactions

Another way to control complexity in the Naming Game is to choose whether to trust or not other agents during a given interaction, by taking into account or not their own word-meaning associations. In previous work, a purely stochastic acceptance of new information has been studied [97]. However, accepting or not new information should depend on the memory provided by past interactions to be efficient. To do so, we use a local approximation of the global agreement as a functional to optimize at each interaction, based on recent information: the LAPS measure 7.1.4.1. We can show that for an appropriate time scale of this recent information, local complexity (amount of word-meaning association to be remembered) remains low, without impacting the duration of the global agreement process. The exact dependance on parameters (time scale, population size, meaning and word spaces size) is still to be explored.

7.1.4.4. Structured meaning spaces exploration
Figure 10. Measures of convergence (global probability of success) and global complexity (number of distinct word-meaning association present in the population) for simulations using Random Topic Choice and MAB LAPS maximization Topic Choice. The active topic choice strategy yields faster convergence, with less complexity. Parameters used: 60 agents, 40 meanings, 40 words, time scale for LAPS 10 interactions.

In the models we have considered so far, meanings were always in a finite number, and without any structure or relative importance. Also, the whole meaning space is accessible from the start. We studied a scenario where meanings are not all available from the beginning, but taken from a growing space: known meanings plus the Adjacent Possible [131] [172]. In practice, we consider a graph of meanings, and a starting meaning $m_0$. The adjacent possible is the set of nodes connected to $m_0$. Whenever a meaning from this set is explored, it is withdrawn from the adjacent possible, but all its neighbors not already known are added to it. In this case, Active Topic Choice helps to keep a quasi-linear pace of exploration, while agreeing on explored meanings. Random Topic Choice explores all available meanings before starting the agreement process: hence, on a big meaning space, possibly infinite, this is really inefficient in terms of communication success. See figure 11.

7.1.4.5. Interactive application for collaborative creation of a language: Experimenting how humans actively negotiate new linguistic conventions

How do humans agree and negotiate linguistic conventions? This question is at the root of the domain of experimental semiotics [118], which is the context of our experiment/application. Typically, the experiments of this field consist in making human subjects play a game where they have to learn how to interact/collaborate through a new unknown communication medium (such as abstract symbols). In recent years, such experiments allowed to see how new conventions could be formed and evolve in population of individuals, shading light on the origins and evolution of languages [133] [116].

We consider a version of the Naming Game [177] [140], focusing on the influence of active learning/teaching mechanisms on the global dynamics. In particular, agreement is reached sooner when agents actively choose the topic of each interaction [49], [60], [61].

Through this experiment, we confront existing topic choice algorithms to actual human behavior. Participants interact through the mediation of a controlled communication system – a web application – by choosing words to refer to objects. Similar experiments have been conducted in previous work to study the agreement dynamics on a name for a single picture [106]. Here, we make several pictures or interaction topics available, and quantify the extent to which participants actively choose topics in their interactions.

- **Individual short experiment (implemented):** Each user interacts for about 3-4 min (<30 interactions) with a brand new population of 7 simulated agents. They take the role of one designated agent, and play the Naming Game as this agent. Each time they interact as speakers, they can select the topics of conversation from a set of 5 objects, and are offered 6 possible words to refer to...
Figure 11. Comparison of Random and Active Topic Choice on a structured meaning space. The space used is a balanced tree, with initially accessible meaning being the root of the tree. On the left, evolution of global complexity (number of distinct word-meaning association present in the population): Active Topic Choice helps keeping a low complexity, with quasi linear growth, whereas Random Topic Choice first goes to a maximum way higher than the final expected value. Parameters used: 10 agents, 100 meanings, 100 words. On the right, illustration of the status of a population in both cases, after half of the interactions needed to converge to global agreement. Nodes represent meanings, their size the number of agents having at least a word for them, and their color the level of agreement between all agents of the population for the given meaning. We can see that Active Topic Choice population has not talked about all meanings, but agrees on all the one that were used; whereas in the other case all meanings were used but almost no agreement is reached.
them. Their choices influence the global emergence of a common lexical convention, reached when communications are successful. The goal is to maximize a score based on the number of successful interactions (among the 50 in total for each run). They can see a list of the past interactions, with chosen topic, chosen word, and whether the interaction was successful or not. This experiment allows us to directly measure if there is a bias in the choice of topics, compared to random choice, based on memory of past interactions. Performance can then be compared to existing topic choice algorithms [49], [60], [61].

- Collective creation of a language and conceptual exploration (under development): Users interact with agents picked from a population which is kept for the whole duration of the experiment, common to all users. Meanings that can be used as topics are drawn from a bigger space than for the first experiment. Word space is a combination of a few basic available syllables (to avoid direct usage of known words). Users interact with a slowly increasing subset of this population, so that newcomers have the same level of influence within their own part of the experiment as people who interacted at the beginning of the day. Successfully communicating about certain meanings/objects unlocks new available meanings, and therefore we can observe the whole process of collective conceptual exploration. Linguistic conventions are set and learned/shared by users, through the interaction with simulated agents. Users never interact directly with each other, therefore no synchronization is needed. In other words, if one user decides not to finish the current interaction, it will not affect other users. We can measure in this scenario statistical properties of the language like frequency distribution, rate of exploration as well as degree of convergence.

![Figure 12. Example of a game with the interface already existing. Play it here: http://naming-game.bordeaux.inria.fr](http://naming-game.bordeaux.inria.fr)

The experiment – available at [http://naming-game.bordeaux.inria.fr](http://naming-game.bordeaux.inria.fr) – was presented at the Kreyon Conference in Rome, in september 2017, during a talk and as part of interactive installation consisting in numerous scientific experiments. Insufficient data was collected to get significant results. To recruit more players and collect a large amount of data, we plan to use crowdsourcing platforms.
7.2. Autonomous Machine Learning and Applications to Developmental Robotics

7.2.1. Intrinsically Motivated Goal Exploration and Multi-Task Reinforcement Learning

Participants: Sébastien Forestier, Pierre-Yves Oudeyer [correspondant], Alexandre Péré, Olivier Sigaud, Pierre Manceron, Yoan Mollard.

7.2.1.1. Intrinsically Motivated Exploration of Spaces of Parameterized Skills/Tasks and Application to Robot Tool Learning

A major challenge in robotics is to learn parametrized policies to solve multi-task reinforcement learning problems in high-dimensional continuous action and effect spaces. Of particular interest is the acquisition of inverse models which map a space of sensorimotor problems to a space of motor programs that solve them. For example, this could be a robot learning which movements of the arm and hand can push or throw an object in each of several target locations, or which arm movements allow to produce which displacements of several objects potentially interacting with each other, e.g. in the case of tool use. Specifically, acquiring such repertoires of skills through incremental exploration of the environment has been argued to be a key target for life-long developmental learning [96].

This year we developed a formal framework called “Unsupervised Multi-Goal Reinforcement Learning”, as well as a formalization of intrinsically motivated goal exploration processes (IMGEPs), that is both more compact and more general than our previous models [89]. We experimented several implementations of these processes in a complex robotic setup with multiple objects 13, associated to multiple spaces of parameterized reinforcement learning problems, and where the robot can learn how to use certain objects as tools to manipulate other objects. We analyzed how curriculum learning is automated in this unsupervised multi-goal exploration process, and compared the trajectory of exploration and learning of these spaces of problems with the one generated by other mechanisms such as hand-designed learning curriculum, or exploration targeting a single space of problems, and random motor exploration. We showed that learning several spaces of diverse problems can be more efficient for learning complex skills than only trying to directly learn these complex skills. We illustrated the computational efficiency of IMGEPs as these robotic experiments use a simple memory-based low-level policy representations and search algorithm, enabling the whole system to learn online and incrementally on a Raspberry Pi 3.

Figure 13. Robotic setup. Left: a Poppy Torso robot (the learning agent) is mounted in front of two joysticks. Right: full setup: a Poppy Ergo robot (seen as a robotic toy) is controlled by the right joystick and can hit a tennis ball in the arena which changes some lights and sounds.
In order to run more scientific experiments in a shorter time, we scaled up this experimental setup to a platform of 6 identical Poppy Torso robots, each of them having the same environment to interact with. Every robot can run a different task with a specific algorithm and parameters each. In this setup Poppy Torso robots are requesting jobs to a dedicated computer acting as a job manager which monitors execution and distributes jobs to available robots. Moreover, each Poppy Torso can also perceive the motion of a second Poppy Ergo robot, which can be used, this time, as a distractor performing random motions to complicate the learning problem. 12 top cameras and 6 head cameras can dump video streams during experiments, in order to record video datasets. Data and videos are stored on-the-fly on 6 hard disks.

Figure 14. Platform of 6 robots with identical environment: joysticks, Poppy Ergo, ball in an arena, and a distractor. The central bar supports the 12 top cameras.

7.2.1.2. Unsupervised Deep Learning of Goal Spaces for Goal Intrinsically Motivated Goal Exploration

Intrinsically motivated goal exploration algorithms enable machines to discover repertoires of policies that produce a diversity of effects in complex environments. These exploration algorithms have been shown to allow real world robots to acquire skills such as tool use in high-dimensional continuous state and action spaces. However, they have so far assumed that self-generated goals are sampled in a specifically engineered feature space, limiting their autonomy. We have proposed an approach using deep representation learning algorithms to learn an adequate goal space. This is a developmental 2-stage approach: first, in a perceptual learning stage, deep learning algorithms use passive raw sensor observations of world changes to learn a corresponding latent space; then goal exploration happens in a second stage by sampling goals in this latent space. We made experiments with a simulated robot arm interacting with an object, and we show that exploration algorithms using such learned representations can closely match, and even sometimes improve, the performance obtained using engineered representations.

7.2.1.3. Combining deep reinforcement learning and curiosity-driven exploration

A major challenge of autonomous robot learning is to design efficient algorithms to learn sensorimotor skills in complex and high-dimensional continuous spaces. Deep reinforcement learning (RL) algorithms are natural candidates in this context, because they can be adapted to the problem of learning continuous control policies with low sample complexity. However, these algorithms, such as DDPG (Lillicrap et al., 2016) suffer from exploration issues in the context of sparse or deceptive reward signals.

In this project, we investigate how to integrate deep reinforcement learning algorithms with curiosity-driven exploration methods. A key idea consists in decorrelating the exploration stage from the policy learning stage by using a memory structure used in deep RL called a replay buffer. Curiosity-driven exploration algorithms, also called Goal Exploration Processes (GEPs) are used in a first stage to efficiently explore the state and action space of the problem, and the corresponding data is stored into a replay buffer. Then a DDPG learns a control policy from the content of this replay buffer.
The internship of Pierre Manceron has been dedicated to trying this methodology in practice. Pierre has combined GEPs obtained from the Explauto open-source library (Moulin-Frier et al., 2014) and his own implementation of DDPG, and benchmarked the combination using the openAI Gym toolkit (Duan et al., 2016).

Preliminary results have revealed some stability issues in DDPG, whereas encouraging results were obtained about the combination with GEPs. Beyond getting more robust results and publishing them, our next goal is to envision other ways to integrate deep RL with curiosity-driven exploration processes by using the tools of the former to more efficiently implement the latter.

7.2.2. Social Learning of Interactive Skills

**Participants:** Manuel Lopes [correspondant], Baptiste Busch, Yoan Mollard, Thibaut Munzer.

This work was made in collaboration with Marc Toussaint and Guilherme Maeda.

7.2.2.1. Preference learning on the execution of collaborative human-robot tasks

One important aspect of the human-robot collaboration is to be able to learn the user’s preferences on the sequence of actions. By querying the user on the next action, when the uncertainty is high, the robot learns the user preferences (Q-function) to solve the task. From a planning point of view, this Q-function can then be integrated into the solver to select the user preferred route to solve a task when multiple choices are available. Therefore, this work aims at reducing the human cognitive load by:

- querying demonstrations only when the uncertainty is above a certain threshold,
- always choose the user preferred actions.

This work has been accepted for publication in the *International Conference on Robotics and Automation (ICRA)* 2017 and presented during the conference [80].

Interestingly, this also raises questions on the robot autonomy and its perception by the human coworker. By interacting with a user, the robot starts to learn the preferred actions and will take initiative to perform them on the next assembly. The question is, how does the user perceives this initiative taking? To answer this question, we have conducted a user study to analyze the impact of robot initiative on the collaboration. Two conditions were considered:

- a semi-autonomous robot that learns and decides when to execute a supporting action,
- a support robot that has to be instructed of each action on a collaborative task.

We found that users prefer the semi-autonomous robot and that the behavior was closer to their expectations despite them being more afraid of it. We also found that even if users noticed the robot was learning in one case, they wanted more autonomy in both conditions. This research was published in the companion of the *Conference on Human-Robot Interaction (HRI)* 2017 and presented during the poster sessions of the conference [82].

7.2.2.2. Learning legible motions from interaction

In a human-robot collaboration context, understanding and anticipating the robot intentions ease the completion of a joint-task. Whereas previous work has sought to explicitly optimize the legibility of behavior, we investigate legibility as a property that arises automatically from general requirements on the efficiency and robustness of joint human-robot task completion.

Following our previous work on legibility of robot motions [64], we have conducted several user experiments to analyze the effects of the policy representation on the universality of the legibility.

This work lead to a submission of a journal article to the *International Journal of Social Robotics (IJSR)* [69].
7.2.2.3. Postural optimization for an ergonomic human-robot interaction

When we, humans, accomplish a task our body posture is (partially) constrained. For example, acting on an object constrains the pose of the hand relatively to the object, and the head faces the object we are acting upon. But due to the large number of degrees of freedom (DOF) of the human body, other body parts are unconstrained and several body postures are viable with respect to the task. However, not all of them are viable in terms of ergonomics. Using a personalized human model, observational postural assessment techniques can be automatized. Optimizing the model body posture is then the logical next step to find an ergonomically correct posture for the worker to accomplish a specific task.

To optimize the subject’s model to achieve a specific task, we define an objective function that minimizes the efforts of the whole body posture, based on the Rapid Entire Body Assessment (REBA) technique [124]. The objective function also account for visibility of the target object and worker’s laterality. We have also implemented an automatic assessment of the worker’s body posture based on the REBA method.

![Image](image.jpg)

*Figure 15. Representation of the setup considered in the user study. The robot presents to the user a spherical ball in which multiple shapes can be inserted. Final pose of the object is calculated from the user posture at his current location. Body motions during the insertion are recorded using a suit made from OptiTrack markers.*

Using a spherical object, carried by a Baxter humanoid robot as illustrated in Fig. 15, we mimic an industrial scenario where the robot helps the worker by positioning and orienting an object in which the worker has to insert specific shapes. In a user-study with forty participants, we compare three different robot’s behaviors, one of them being the result of the postural optimization of the subject’s personalized model. By the mean of a survey session, and the online assessment of the subject’s posture during the interaction, we prove that our method leads to a safer posture, and is perceived as more comfortable.

This work has been published to the International Conference on Intelligent Robots and Systems (IROS) [75] and was presented during the conference.

7.2.2.4. Planning ergonomic sequences of actions in human-robot interaction

Following our work on physical ergonomics [75], we have extended our method to include it in the Logic-Geometric Program (LGP) [171]. This method allows us to solve Task and Motion Planning (TAMP) problems simultaneously while optimizing for maximum ergonomics on the human side.

In a simulated experimented we prove that the solver is able to choose the logic actions (e.g. “the robot places the screwdriver on the table”) that provides maximum ergonomics throughout the interaction. By the mean of an experiment on our Baxter robot, we also prove that optimizing ergonomics over the full sequences of actions, as opposed to the step-wise approach we were considering in [75] where ergonomics was optimized for single atomic actions, lead to a more ergonomic interaction.
As both human and robot agents are capable of performing the same task, this creates a need to communicate the planned sequence of actions efficiently to the human. Two problems are raised by this dynamic task allocation. First, the human need to understand the current action performed by the robot to anticipate and react if necessary. Second, the human must know beforehand or during the executions the actions that he or she has to perform and when to perform them.


![Image](image.png)

The robot, using its left arm, hands over the toolbox handle to the agent's right hand.

**Figure 16.** A representation of an action generated by the solver and displayed on a webpage to simplify the visualization. The agent can click on the image to start a video of the action. Arrows on the right corner are also clickable to navigate between the previous and the next actions.

To this purpose, we also introduce a graphical interface that displays the current action and the geometric of the scene as illustrated in figure 16. This graphical interface can be used offline to train the human on the steps required for the whole task. It can also be displayed online to show the current action to reduce the human cognitive load of understanding the action performed by the robot and understanding the action that he or her is expected to perform.

This work was submitted to the International Conference on Robotics and Automation (ICRA) and is currently under review.

7.2.2.5. Active incremental learning of robot movement primitives

A robot coworker acting as a third hand brings the challenge that its skills must be augmented and tailored as needed, over time. To this end, imitation learning can rely on the presence of the human coworker as a teacher. However, imitation learning has primarily addressed how to endow and refine robots with motor skills but not when the learning should take place. Reasoning when improvement is actually needed is, nevertheless, an essential and difficult problem to be solved. We propose an active learning algorithm that allows a robot to reason about the confidence of its movement primitives. It allows the robot to decide when a demonstration is required, making active requests to the human coworker depending on its confidence.

This capability also sheds light onto the problem of deciding how many demonstrations are needed to construct a probabilistic model when learning from demonstrations. Under active learning, the number of demonstrations is indicated by the robot, on-demand. The method can be used on a single demonstration, in a one-shot learning fashion. If the extrapolation is, however, beyond the scope of the existing demonstration—indicated by the uncertainty—an active request will be made. The proposed method also offers a principled way to train Dynamical Movement Primitives (DMPs) with contextualized demonstrations encoded by Gaussian Processes (GPs)—details can be found in [79].
The method is based on a combination of GPs and DMPs, where the former provides the confidence bounds in which the demonstrations are being extrapolated, and the latter accounts for prediction errors due to the nonlinearities of the function being approximated. Algorithm 17 shows a pseudocode of the proposed method.

Figure 18 shows the decrease of the uncertainty on the prediction of 10 trajectories as the number of demonstrations increase (the ellipses represent the projections of one standard deviation along the trajectory). Figure 18(a)(b) and (c) show the predictions after one, two and five demonstrations, respectively. The blue color in (c) indicates that the robot has confidence it can execute the 10 predicted trajectories.

7.3. Representation Learning

7.3.1. Cross-situational noun and adjective learning in an interactive scenario

Participants: David Filliat [correspondant], Yuxin Chen.

Future intelligent robots are expected to be able to adapt continuously to their environment. For this purpose, recognizing new objects and learning new words through interactive learning with humans is fundamental. Such setup results in ambiguous teaching data which humans have been shown to address using cross-situational learning, i.e. by analyzing common factors between multiple learning situations. Moreover, they have been shown to be more efficient when actively choosing the learning samples, e.g. which object they want to learn. Implementing such abilities on robots can be performed by latent-topic learning models such as Non-Negative Matrix Factorization or Latent Dirichlet Allocation. These cross-situational learning methods tackle referential and linguistic ambiguities, and can be associated with active learning strategies. We propose two such methods: the Maximum Reconstruction Error based Selection (MRES) and Confidence Base Exploration (CBE). We present extensive experiments using these two learning algorithms through a systematic analysis on the effects of these active learning strategies in contrast with random choice. In addition, we study the factors underlying the active learning by focusing on the use of sample repetition, one of the learning behaviors that have been shown to be important for humans. These results have been published in a journal paper [70].
Figure 18. Decrease of the trajectory uncertainties as demonstrations for objects are being requested. The ellipses show a single standard deviation. Uncertainties above the threshold are shown in red. The blue trajectories indicate that the robot is confident in executing the primitives. (a) The uncertainties for all contexts after one demonstration. (b) Predictions after two demonstrations. (c) Predictions after five demonstrations.

7.3.2. State Representation Learning in the Context of Robotics

Participants: David Filliat [correspondant], Natalia Diaz Rodriguez, Timothee Lesort, Mathieu Seurin.

Our understanding of the world depends highly on our capacity to produce intuitive and simplified representations which can be manipulated and combined easily to solve problems. We worked on reproducing this simplification process using a neural network to build a low dimensional state representation of the world from images acquired by a robot. As in the approach from Jonschkowski [129], we learn in an unsupervised way using prior knowledge about the world as loss functions called robotic priors.

The robotic priors loss function impose constraint in a low dimension space. We call this space the representation space and it contains the underlying parameters of the robot environment. This constraint are physic related as the time coherence of the representation, the repeatability, the proportionality and causality of the actions inside the representation space.

Imposing those constraint to sequences of images makes it possible to learn a mapping from image to our representation state space. We extend the previous approach to high dimension richer images to learn a 3D representation of the hand position of a robot from RGB images.

We propose a quantitative evaluation of the learned representation using nearest neighbors in the state space that allows to assess its quality and show both the potential and limitations of robotic priors in realistic environments. We augment image size, add distractors and domain randomization, all crucial components to achieve transfer learning to real robots.

Finally, we also contribute a new prior to improve the robustness of the representation. This prior takes profit of the initial state of the robot to bring together representation of different sequences. The applications of such low dimensional state representation range from easing reinforcement learning (RL) and knowledge transfer across tasks, to facilitating learning from raw data with more efficient and compact high level representations.

Our experiments [90] (see figure 19 for an illustration) compare results in different setup with state representation in 2 and 3D, with different amount of distractors. The results show that the robotic prior approach is able to extract high level representation such as the 3D position of an arm and organize it into a compact and coherent space of states in a challenging dataset.
7.3.3. Transfer Learning from Simulated to Real World Robotic Setups

Participants: Florian Golemo [correspondant], Pierre-Yves Oudeyer.

This work was made in collaboration with Adrien Ali Taiga and Aaron Courville. Reinforcement learning with function approximation has demonstrated remarkable performance in recent years. Prominent examples include playing Atari games from raw pixels, learning complex policies for continuous control, or surpassing human performance on the game of Go. However most of these successes were achieved in non-physical environments (simulations, video games, etc.). Learning complex policies on physical systems remains an open challenge. Typical reinforcement learning methods require a lot of data which makes it unsuitable to learn a policy on a physical system like a robot, especially for dynamic tasks like throwing or catching a ball. One approach to this problem is to use simulation to learn control policies before applying them in the real world. This raises new problems as the discrepancies between simulation and real world environments ("reality gap") prevent policies trained in simulation from performing well when transferred to the real world. This is an instance of domain adaption where the input distribution of a model changes between training (in simulation) and testing (in real environment). The focus of this work is in settings where resetting the environment frequently in order to learn a policy directly in the real environment is highly impractical. In these settings the policy has to be learned entirely in simulation but is evaluated in the real environment, as zero-shot transfer.

In simulation there are differences in physical properties (like torques, link weights, noise, or friction) and in control of the agent, specifically joint control in robots. We propose to compensate for both of these source of issues with a generative model to bridge the gap between the source and target domain. By using data collected in the target domain through task-independent exploration we train our model to map state transitions from the source domain to state transition in the target domain. This allows us to improve the quality of our simulated robot by grounding its trajectories in realistic ones. With this learned transformation of simulated trajectories we are able to run an arbitrary RL algorithm on this augmented simulator and transfer the learned policy.
directly to the target task. We evaluate our approach in several OpenAI gym environments that were modified to allow for drastic torque and link length differences.

7.3.4. Measuring Uncertainty in Deep Learning Networks

**Participants:** Florian Golemo [correspondent], Manuel Lopes.

As precursor to the main objective of the IGLU project, we investigated methods that would enable deep neural networks to judge their knowledge about a domain.

Neural networks, especially deep ones, have been shown to be able to model arbitrarily complex problems, and thus offer powerful tools for machine learning. Yet they come with a significant flaw of not being inherently able to represent certainty of their predictions. By adding a measure of uncertainty to neural networks, this technology could be applied to autonomous exploration and open-ended learning tasks.

Thus the goal of this project was to find a method to measure how much knowledge a neural network has about an unlabeled data item (measure of uncertainty), and to apply this new measure in an active learning context. The objective of the latter was to demonstrate the efficiency in handpicking interesting data, to optimally extend the system’s own capabilities.

We were successful in finding a measure of uncertainty that would reliably distinguish data that the network has seen before, from data that was generally unfamiliar to the network. This measure was created by measuring the entropy of the network’s last layer across a batch of stochastic samples generated by adding Poisson noise to the inputs.

The measure failed however to outperform random sampling in several active learning scenarios. Yarin Gal published related work as part of his dissertation [117] after this project was concluded. He elaborated that deep neural networks are very effective in canceling out input noise. The author suggested to use existing “Dropout” layers instead for stochastic sampling, but he reaches the same conclusion of using the last layer entropy as measure of uncertainty.

7.4. Applications in Robotic myoelectric prostheses

**Participants:** Pierre-Yves Oudeyer [correspondent], Manuel Lopes, Mathilde Couraud, Sebastien Mick, Aymar de Rugy, Daniel Cattaert, Florent Paclet.

Together with the Hybrid team at INCIA, CNRS, the Flowers team continued to work on establishing the foundations of a long-term project related to the design and study of myoelectric robotic prosthesis. The ultimate goal of this project is to enable an amputee to produce natural movements with a robotic prosthetic arm (open-source, cheap, easily reconfigurable, and that can learn the particularities/preferences of each user).

This will be achieved by 1) using the natural mapping between neural (muscle) activity and limb movements in healthy users, 2) developing a low-cost, modular robotic prosthetic arm and 3) enabling the user and the prosthetic system to co-adapt to each other, using machine learning and error signals from the brain, with incremental learning algorithms inspired from the field of developmental and human-robot interaction.

7.4.1. Model and experiments to optimize co-adaptation in a simplified myoelectric control system

To compensate for a limb lost in an amputation, myoelectric prostheses use surface electromyography (EMG) from the remaining muscles to control the prosthesis. Despite considerable progress, myoelectric controls remain markedly different from the way we normally control movements, and require intense user adaptation. To overcome this, our goal is to explore concurrent machine co-adaptation techniques that are developed in the field of brain-machine interface, and that are beginning to be used in myoelectric controls. We combined a simplified myoelectric control with a perturbation for which human adaptation is well characterized and modeled, in order to explore co-adaptation settings in a principled manner. First, we reproduced results obtained in a classical visuomotor rotation paradigm in our simplified myoelectric context, where we rotate the muscle pulling vectors used to reconstruct wrist force from EMG. Then, a model of human adaptation in response to directional error was used to simulate various co-adaptation settings, where perturbations and machine co-adaptation are both applied on muscle pulling vectors. These simulations
established that a relatively low gain of machine co-adaptation that minimizes final errors generates slow and incomplete adaptation, while higher gains increase adaptation rate but also errors by amplifying noise. After experimental verification on real subjects, we tested a variable gain that cumulates the advantages of both, and implemented it with directionally tuned neurons similar to those used to model human adaptation. This enables machine co-adaptation to locally improve myoelectric control, and to absorb more challenging perturbations. Significance. The simplified context used here enabled to explore co-adaptation settings in both simulations and experiments, and to raise important considerations such as the need for a variable gain encoded locally.

This work was published in the Journal Of Neural Engineering in [71]

7.4.2. Performance and Usability of Various Robotic Arm Control Modes from Human Force Signals

Elaborating an efficient and usable mapping between input commands and output movements is still a key challenge for the design of robotic arm prostheses. In order to address this issue, we developed and compared three different control modes, by assessing them in terms of performance as well as general usability. Using an isometric force transducer as the command device, these modes convert the force input signal into either a position or a velocity vector, whose magnitude is linearly or quadratically related to force input magnitude. With the robotic arm from the open source 3D-printed Poppy Humanoid platform simulating a mobile prosthesis, an experiment was carried out with eighteen able-bodied subjects performing a 3-D target-reaching task using each of the three modes. The subjects were given questionnaires to evaluate the quality of their experience with each mode, providing an assessment of their global usability in the context of the task. According to performance metrics and questionnaire results, velocity control modes were found to perform better than position control mode in terms of accuracy and quality of control as well as user satisfaction and comfort. Subjects also seemed to favor quadratic velocity control over linear (proportional) velocity control, even if these two modes did not clearly distinguish from one another when it comes to performance and usability assessment. These results highlight the need to take into account user experience as one of the key criteria for the design of control modes intended to operate limb prostheses. This work was published in the journal Frontiers in Neurorobotics [72].

7.5. Applications in Educational Technologies

7.5.1. Machine Learning for Adaptive Personalization in Intelligent Tutoring Systems

**Participants:** Manuel Lopes [correspondant], Pierre-Yves Oudeyer, Didier Roy, Alexandra Delmas, Benjamin Clement.

7.5.1.1. The Kidlearn project

Kidlearn is a research project studying how machine learning can be applied to intelligent tutoring systems. It aims at developing methodologies and software which adaptively personalize sequences of learning activities to the particularities of each individual student. Our systems aim at proposing to the student the right activity at the right time, maximizing concurrently his learning progress and its motivation. In addition to contributing to the efficiency of learning and motivation, the approach is also made to reduce the time needed to design ITS systems.

We present an approach to Intelligent Tutoring Systems which adaptively personalizes sequences of learning activities to maximize skills acquired by students, taking into account the limited time and motivational resources. At a given point in time, the system proposes to the students the activity which makes them progress faster. We introduce two algorithms that rely on the empirical estimation of the learning progress, **RIARIT** that uses information about the difficulty of each exercise and **ZPDES** that uses much less knowledge about the problem.
The system is based on the combination of three approaches. First, it leverages recent models of intrinsically motivated learning by transposing them to active teaching, relying on empirical estimation of learning progress provided by specific activities to particular students. Second, it uses state-of-the-art Multi-Arm Bandit (MAB) techniques to efficiently manage the exploration/exploitation challenge of this optimization process. Third, it leverages expert knowledge to constrain and bootstrap initial exploration of the MAB, while requiring only coarse guidance information of the expert and allowing the system to deal with didactic gaps in its knowledge. The system is evaluated in a scenario where 7-8 year old schoolchildren learn how to decompose numbers while manipulating money. Systematic experiments are presented with simulated students, followed by results of a user study across a population of 400 school children. [14]

7.5.1.2. Linear UCB for intelligent tutoring system

What we wanted to do was to use the feature space considering features of students, features of explanations and maybe feature about the exercises. We wanted use this feature space to guide the bandit algorithm to recommend explanations. The algorithms that we already developed cannot be used in this kind of problem, because the order and the value of the bandit values depends on the time and on the learning progress the actions give in time. And in this new experiment, we wanted to recommend feedback, base on the population results depending on student’s and explanation’s features. In this problem, there is no consideration about temporality and the long-term progression of the student is too hard to correlate with a particular explanation. So different algorithms have been studied in the literature to use contextual bandit to make recommendation over a population. The algorithm that we wanted to use and adapt to our purpose is the LinUCB algorithm from [136].

Different kind of simulation have been made to test this framework. These experiments were made by generating various population of student defined by binary features with a number of dimension between 5 and 20. Also a set of activity have been defined and depending of the features of the students, their result for each activity was right or wrong. The algorithm was trained by making the student work on random activities, this way, the algorithm would learn the correlation between the student feature space and the success/failure to activities. After that the tests was made by letting the algorithms to choose the activity to propose to the student depending of their features. A lot of different configurations have been tested. The algorithm showed good results for low dimension feature space (3 to 9 features) with 90% accuracy, but for high dimension feature space, the results dropped to 20-30% accuracy.

7.5.1.3. Experiment in class in 2018

An experiment will be held in mars 2018 about testing the kidlearn framework in classroom in Bordeaux Metropole. The goal is to test a new feature by giving the student the opportunity to have different kinds of choice. This choice would be managed by a multi-armed bandit algorithm. We want to make an experiment with 600 student from bordeaux Metropole and we are currently discussing with the Local Education Authority to also test the application in other school in other departments.

7.5.1.4. The KidBreath project

To create learning contents linked to asthma to personalize it like mathematics activities in Kidlearn project [14] we used recomendation criterias in Therapeutic Education Program for asthma kids made by Health High Autority. Following an approach of participatory design [102], contents were validated by medical experts like health educators, pulmonologists and pediatrics. Then, we conducted a workshop with forty kids aged 8 in order to iterate over the application interfaces and evaluate enjoy about it with observations. Finally, we realized a focus group with 5 asthma kids to validate the global comprehension of a part of the content. It revealed that children wanted more contents about the crisis treatment and how the asthma works in the human system (verbatim).

In a preliminary study, we experimented the participatory design process (PD) in the context of asthma e-learning using KidBreath tool. We evaluated in two Year 4 classes its efficacy in a motivation way [175], usability [142], [157], disease knowledge [92] and interests of children by their system [119]. After two weeks a use, results showed, in acceptance with behaviors, high level of intrinsic motivation when using KidBreath, usability and enjoyment of edutainment activities. This pilot study tends to confirm to continue with this
approach with asthma kids at home (study in progress). These results was presented in the 29st Conference in Computer-Human Interaction in Poitiers, France.

We presented Thesis project in some events this year, with one publication surbmitted and validated:

- 21ème Congrès de Pneumologie de la Langue Française, January 2017, Marseille, France (Poster)
- Journée IIM et IA, March 2017, Paris, France (oral presentation)
- Ma Thèse en 180 secondes, March 2017, Bordeaux, France (oral presentation),
- 29ème conférence francophone sur l’Interaction Homme-Machine, August 2017, Poitiers, France (article and oral presentation) [76],
- La nuit européenne des chercheurs, September 2017, Bordeaux, France (oral presentation).

7.5.2. Poppy Education: Designing and Evaluating Educational Robotics Kits

Participants: Pierre-Yves Oudeyer [correspondant], Didier Roy, Théo Segonds, Stéphanie Noirpoudre, Thibault Desprez, Damien Caselli, Aurélie Lopes, Kelian Schindowsky.

Poppy Education project aims to create, evaluate and disseminate all-inclusive pedagogical kits, open-source and low cost, for teaching computer science and robotics. It is designed to help young people to take ownership with concepts and technologies of the digital world, and provide the tools they need to allow them to become actors of this world, with a considerable socio-economic potential. It is carried out in collaboration with teachers and several official french structures (French National Education, High schools, engineer schools, ... ). For secondary education and higher education, scientific literacy centers, Fablabs.

Poppy Education is based on the robotic platform poppy (open-source platform for the creation, use and sharing of interactive 3D printed robots), including:

- Poppy Humanoid, a robust and complete robotics platform designed for genuine experiments in the real world and can be adapted to specific user needs.
- Poppy Torso, a variant of Poppy Humanoid that can be easily installed on any flat support.
- Ergo Jr, a robotic arm. Durable and inexpensive, it is perfect to be used in class. Python. Directly from a web browser, using Ipython notebooks (an interactive terminal, in a web interface for the Python Programming Language).
- Snap. The visual programming system Snap, which is a variant of Scratch. Its features allow a thorough introduction of information technology.
- C++, Java, Matlab, Ruby, Javascript, etc. thanks to a REST API that allows you to send commands and receive information from the robot with simple HTTP requests.
- Virtual robots (Poppy Humanoid, Torso and Ergo) can be simulated with the free simulator V-REP. It is possible in the classroom to work on the simulated model and then allow students to run their program on the physical robot.

7.5.2.1. Pedagogical experimentations : Design and experiment robots and the pedagogical activities in classroom.

This project is user centered design. The pedagogical tools of the project (robots and ressources) are being created directly with the users and evaluated in real life by experiments. So teachers and researchers co-creatie activities, test with students in class-room, exchange their uses and develop the platform as needed [81]. The activities were designed mainly with Snap! and Python. Most activities use Poppy Ergo Jr, but some use Poppy Torso (mostly in higher school because of its cost).
Figure 20. Experiment robots and pedagogical activities in classroom

The pedagogical experiments in classroom carried out during the first year of the project notably allowed to create and experiment many robotic activities and to create pedagogical resources to taking in hand the robot. The main objective of the second year was to make all the activities and resources reusable (with description, documentation and illustration) easily and accessible while continuing the experiments and the diffusion of the robotic kits.

- Pedagogical working group: in the second year, the teacher partners continued to use the robots in the classroom and to create and test new classroom activities. Four new schools (including 10 new teachers) from different backgrounds (middle-school and high school teachers) have been added to the group to add diversity. We organized some training to help them to discover and learn how to use the robotics platform. As well an engineer of the Poppy Education team went to visit the teachers in their school to see and to evaluate the pedagogical tools (robots and activities) in real contexts of use.

Five meetings have been organized during the year will all teachers partners and Poppy Education team to exchange about their projects with robots, to understand their need and to get some feedbacks from them. This experimentations are still helping us to understand better the educational needs, to create and improve the pedagogical tools.

You can see the videos of pedagogical robotics activities here: https://www.youtube.com/playlist?list=PLdX8RO6QsgB7hM_7SQNLvyp2QiDAkkzLn

7.5.2.2. Pedagogical documents and resources

- We continued to improve the documentation of the robotic platform Poppy (https://docs.poppy-project.org/en/) and the documentation has been translated into French (https://docs.poppy-project.org/fr/).

We configured a professional platform to manage the translation of the documentation (https://crowdin.com/project/poppy-docs). This allow whoever wants to participate in the translation of the language of their choice.

- To complete the pedagogical booklet [48] that provides guided activities and small challenges to become familiar with Poppy Ergo Jr robot and the Programming language Snap! (https://drive.google.com/file/d/0B2jV8vVX-TUxXZjF3OGxHVGM/view) we provided a list of Education projects. Educational projects have been written for each activity carried out and tested in class. So each projects have its own web page including resources allowing any other teacher to carry out the
activity (description, pedagogical sheet, photos/videos, pupil’s sheet, teacher’s sheet with correction etc.).
You can see the activities here:
https://www.poppy-education.org/activites/activites-lycee
The pedagogical activities are also available on the Poppy project forum where everyone is invited to comment and create new ones:
https://forum.poppy-project.org/t/liste-dactivites-pedagogiques-avec-les-robots-poppy/2305

Figure 21. Open-source educational activities with Poppy robots are available on Poppy-Education.org

- A FAQ have been written with the most frequents questions to help the users: https://www.poppy-education.org/aide/

7.5.2.3. Diffusion

- A website have been created to present the project and to share all resources and activities. https://www.poppy-education.org/
- A press release was issued to announce the poppy education website release. https://www.inria.fr/actualite/mediacenter/poppy-education-la-robotique-pedagogique-s-enrichit-d-un-nouveau-site?mediego_ruuid=09f6a0c0-2ab3-11e7-a75f-fd895fe51065
- To promote educational uses of the platform, we participated in events (conference, seminar etc.). We participated as well at some workshops to introduce students to robotics and programming. See the chapter “popularization” to know the whole list.
- We sent 6 newsletters https://us13.campaign-archive.com/home/?u=17b6815514db7361fc260e0ce&id=95e9e13ae2.
- We wrote blog articles to describe workshops/activities and give feedback from experiences. https://www.poppy-education.org/

7.5.2.4. Symposium robotics

We organized a symposium robotics for the third year (http://dm1r.fr/colloque-robotique-education/) that present research results and feedback on the use of Poppy and Thymio robots in education (other robots have been discussed as well). Poppy Education team and the working group teachers helped with the organisation of the event and during the event (talk and workshops).
7.5.2.5. Evaluate the pedagogical kits

After experimenting and creating tools with educational activities in class and for the class, it is now to evaluate qualitatively and quantitatively the impact of these tools. We must therefore assess, at first, if these tools offer good usability (i.e. effectiveness, efficiency, satisfaction). Then, in a second step, select items that can be influenced by the use of these tools. For example, students’ representations of robotics, their motivation to perform this type of activity, or the evolution of their skills in these areas. In 2017 we conducted experiments to evaluate the usability of kits. We also collected data on students’ perceptions of robotics.

- Population

Our sample is made up of 28 teachers and 146 students from the "New Aquitaine" region who completed survey (online) during the month of June 2017. Here, we study several groups of individuals: teachers and students. Among the students we are interested in those who practiced classroom activities with the Ergo Jr kit during the school year 2016 - 2017 (N = 68) (age = 16, S = 2, 44), 37 are from section "Computer Science and Digital Sciences" (BAC S option ISN), 12 of section "Computer and Digital Creation" (BAC S option ICN) and 18 of the middle School. His 68 students are then divided into different modalities according to the characteristics of the activities they have followed: they may have declared using the educational booklet provided in the kit (N = 13) or not (N = 55) ; have used other robotic kits (N = 16) have practiced less than 6 hours of activity with the robot (N = 30), between 6 and 25 hours (N = 22) or more than 25 hours (N = 16); having built the robot (N = 12); have used the visual programming language Snap! (N = 46), the language of Python textual programming (N = 21), both (N = 8) or none (N = 9), it should be noted that these two languages are directly accessible via the main interface of the robot.

- Evaluation of the tool

We have selected two standardized survey dealing with this issue: SUS (The Systeme Usability Scales) [103] and The AttrakDiff [135]. These two survey are complementary and allow to identify the design problems and to account for the perception of the user during the activities. The results of these are available in the article (in French) [77] publish in the conference Didapro (Lausanne Feb, 2018). Figures 22 and 23 show the averages of the 96 respondents (68 students + 28 teachers) for each of the 10 statements from the SUS and 28 pairs of antonyms to be scored on a scale of 1 to 5 and a 7-point scale, respectively.

![Figure 22. Result of SUS survey](image)

- Evaluation of impact on learner
One of the objectives of the integration of digital sciences in school is to allow students to have a better understanding of the technological tools that surround them daily (i.e. web, data, algorithm, connected object, etc.). So, we wanted to measure how the practice of activities with ErgoJr robot had changed this apprehension; especially towards robots. For that, we used a standardized survey: "attitude towards robot" EuroBarometer 382 originally distributed in 2012 to more than 1000 people in each country of the European Union. On the one hand, we sought to establish whether there had been a change in response between 2012 and 2017, and secondly whether there was an impact on the responses of 2017 according to the participation, or not, in educational activities with ErgoJr robot. The analysis of the results is in progress and will be published in 2018.

### Partnership on education projects

- **Ensam**

  The Arts and Métiers campus at Bordeaux-Talence in partnership with Inria wishes to contribute to its educational and scientific expertise to the development of new teaching methods and tools. The objective is to develop teaching sequences based on a project approach, relying on an attractive multidisciplinary technological system: the humanoid Inria Poppy robot.

  The humanoid Inria Poppy robot offers an open platform capable of providing an unifying thread for the different subjects covered during the 3-years of the Bachelor training: mechanics, manufacturing (3D printing), electrical, mecha-tronics, computer sciences, design.

  Last year students of "bachelor degree" (ENSAM-Talence) have designed, manufactured, assembled and programmed 4 different solutions to replace the fixed hand of Poppy by a gripper device: https://www.youtube.com/watch?v=DZjGaJk2fQk. For the second year, students of "bachelor degree" have designed Wheels for Poppy Torso. https://www.poppy-education.org/2017/06/19/des-roues-pour-poppy-torso-2eme-edition-du-projet-etudiant-de-lensam

- **Poppy entre dans la danse** (Poppy enters the dance)

  The project "Poppy enters the dance" (Canope 33) took place for the second year. It uses the humanoid robot Poppy. This robot is able to move and experience the dance. The purpose of this project is to allow children to understand the interactions between science and choreography, to play with the random and programmable, to experience movement in dialogue with the machine. At the beginning of the project they attended two days of training on the humanoid robot (Inria -
During the project, they met the choreographer Eric Minh Cuong Castaing and the engineer Segonds Theo (Inria - Poppy Education).

You can see a description and an overview of the project here: https://www.youtube.com/watch?v=XfxXaq899kY

7.5.3. IniRobot: Educational Robotics in Primary Schools

Participants: Didier Roy [correspondant], Pierre-Yves Oudeyer.

IniRobot (a project done in collaboration with EPFL/Mobsya) aims to create, evaluate and disseminate a pedagogical kit which uses Thymio robot, open-source and low cost, for teaching computer science and robotics.

IniRobot Project consists to produce and diffuse a pedagogical kit for teachers and animators, to help to train them directly or by the way of external structures. The aim of the kit is to initiate children to computer science and robotics. The kit provides a micro-world for learning, and takes an enquiry-based educational approach, where kids are led to construct their understanding through practicing an active investigation methodology within teams. It is based on the use of the Thymio II robotic platform. More details about this projects were published in RIE 2015 [50] , which presents the detailed pedagogical objectives and a first measure of results showing that children acquired several robotics-related concepts. See also http://www.inirobot.fr.


7.5.3.1. Partnership

The project is carried out in main collaboration with the LSRO Laboratory from EPFL (Lausanne) and others collaborations with French National Education/Rectorat d’Aquitaine, with Canopé Educational Network, with ESPE (teacher’s school) Aquitaine, ESPE Martinique, ESPE Poitiers, National Directorate of Digital Education

7.5.3.2. Created pedagogical documents and resources

- Inirobot pedagogical kit [24]: This pedagogical booklet provides activities scenarized as missions to do. An update of Inirobot pedagogical kit : https://dm1r.inria.fr/uploads/default/original/1X/70037bdd5c290e48c7ec4cb4f26f0e426a4b4c6f6.pdf Another pedagogical booklet has been also created by three pedagogical advisers for primary school, with pedagogical instructions and aims, under ou supervision. new pedagogical kit is available, "Inirobot Scolaire, Langages et robotique", which extends Inirobot in a full primary school approach. http://tice33.ac-bordeaux.fr/Ecolien/ASTEP/tabid/5953/language/fr-FR/Default.aspx
Inirobot website and forum https://dm1r.inria.fr/inirobot or http://www.inirobot.fr With this website, teachers, animators and general public can download documents, exchange about their use of inirobot’s kit.


7.5.3.3. Scientific mediation
Inirobot is very popular and often presented in events (conferences, workshops, ...) by us and by others.

7.5.3.4. Symposium robotics
With Poppy Education, Inirobot is a main line in our colloquium "Robotics and Education" (http://dm1r.fr/)

7.5.3.5. Spread of Inirobot activities
Inirobot activities are inside several projects : Dossier 123 codez from Main à la Pâte Fundation, Classcode project, ...

7.5.3.6. Future MOOC Thymio
A new project is coming, MOOC Thymio, in collaboration with Inria Learning Lab and EPFL (Lausanne, Switzerland), on FUN platform and edX EPFL Platform.) To teach how to use Thymio robot in education.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Autonomous Driving Commuter Car
Participants: David Filliat [correspondant], Emmanuel Battesti.

We further developed a planning algorithm for a autonomous electric car for Renault SAS in the continuation of the previous PAMU project. We improved our planning algorithm in order to go toward navigation on open roads, in particular with the ability to reach higher speed than previously possible, deal with more road intersection case (roundabouts), and with multiple lane roads (overtake, insertion...).

8.2. Bilateral Grants with Industry

8.2.1. Adaptive device for disease awareness and treatment adherence of asthma in children
Participants: Manuel Lopes [correspondant], Alexandra Delmas, Pierre-Yves Oudeyer.

Financing of the CIFRE PhD grant of Alexandra Delmas by Itwell with the goal of developing a tool for self-learning for patients to improve their compliance to treatment.
9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Poppy Education

Poppy Education
Program: Feder - Région Aquitaine
Duration: January 2014 - December 2017
Coordinator: PY Oudeyer, Inria Flowers
Partners: Inria Flowers
Funding: 1 million euros (co-funded by Feder/EU Commission, Region Aquitaine and Inria)

Poppy Education aims to create, evaluate and disseminate pedagogical kits “turnkey solutions” complete, open-source and low cost, for teaching computer science and robotics. It is designed to help young people to take ownership with concepts and technologies of the digital world, and provide the tools they need to allow them to become actors of this world, with a considerable socio-economic potential. It is carried out in collaboration with teachers and several official french structures (French National Education/Rectorat, Highschools, engineering schools, ... ). It targets secondary education and higher education, scientific literacy centers, Fablabs.

Poppy robotic platform used in the project is free hardware and software, printed in 3D, and is intended primarily for:
- learning of computer science and robotics,
- introduction to digital manufacturing (3D printing ...)
- initiation to the integration of IT in physical objects in humanoid robotics, mechatronics.
- artistic activities.

Educational sectors covered by the project are mainly: Enseignement d’exploration ICN en seconde, enseignement ISN en terminale S et bientôt en 1ère , filière STI2D, MPS seconde. Web: http://www.poppy-project.org/education.

9.1.1.1. Perseverons Project

The Perseverons project (Perseverance with / by digital objects), carried by the university via the ESPE (Higher School of Teaching and Education) of Aquitaine, and by the Rectorate of Bordeaux via the DANE (Academic Delegation digital education), aims to measure the real effectiveness of digital techniques in education to improve school motivation and perseverance, and, in the long term, reduce dropout. The project proposes to analyze the real effects of the use of two types of objects, robots, tablets, by comparing the school and non-school contexts of the fablabs. He is one of the 22 winners http://www.gouvernement.fr/efran-les-22-laureats of the “E-Fran” call for projects (training, research and digital animation spaces), following the Monteil mission on digital education, as part of the Investissement d’Avenir 2 program http://ecolenumerique.education.gouv.fr/2016/09/23/1244/ . Formed of 12 sub-projects, "perseverons” has many partnerships, especially with the Poppy Education project http://perseverons.espe-aquitaine.fr/sp6-robotique-inria/.

9.1.1.2. Partner schools

In 2017, we have 36 partner schools (show Fig 25). 15 directly from the Poppy Education project. 19 new establishments were equipped in September 2017 by the Perseverons project. 21 of these establishments are located in Gironde. We have 27 high schools, 5 middle school.

9.1.2. ENSAM

The orientation of a (high school) student, choosing a career, is often based on an imagined representation of a discipline, sector of activity or training. Moreover, higher education is sometimes for a college student or a student a self centered universe, with inaccessible teaching methodologies and level of competence.
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<td>Poppy Education Middle School</td>
<td>Jean Zay</td>
<td>41 Rue Henri Cochet, 33318 Biganos, France</td>
<td>+33 5 57 17 07 70</td>
<td><a href="http://lycee-lamorlette.fr">http://lycee-lamorlette.fr</a></td>
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<tr>
<td>Poppy Education High School</td>
<td>La Molette</td>
<td>2 Rue du Docteur Roux, 33150 Cenon, France</td>
<td>+33 5 57 80 37 00</td>
<td><a href="http://lycee-lamolette.fr">http://lycee-lamolette.fr</a></td>
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<td>PERSEVERONS High School</td>
<td>Les Iris</td>
<td>29 Rue Soubirou, 33130 Lormont, France</td>
<td>+33 5 57 80 10 60</td>
<td><a href="http://www.lyceelesiris.fr">http://www.lyceelesiris.fr</a></td>
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<tr>
<td>PERSEVERONS High School</td>
<td>Louis Barbou</td>
<td>2 Boulevard Barbaregne, 64000 Pau, France</td>
<td>+33 5 59 08 00 00</td>
<td><a href="http://www.cyberlycees.fr">http://www.cyberlycees.fr</a></td>
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<tr>
<td>PERSEVERONS High School</td>
<td>Louis de Poix</td>
<td>4 Avenue Jean Rostand, 84110 Avignon, France</td>
<td>+33 5 59 63 31 10</td>
<td><a href="http://www.lyciedepoix.com">http://www.lyciedepoix.com</a></td>
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| PERSEVERONS High School | Main de Biran | 108 Rue Valette, 24100 Bergerac, France | +33 5 53 74 50 00 | http://webtab.ac-bordeaux.fr/lycee-main-de-biran />
| Poppy Education Middle School | Mios | Route du Puejou, 33380 Mios, France | +33 5 56 03 00 77 | http://www.elycienfance-jeunessecollege.com/lyceemios |
| PERSEVERONS High School | Nord Bassin | 128 Avenue de Bordeaux, 33510 Andermont-les-Bains, France | +33 5 56 62 20 77 | http://www.lyceenordbassin.com |
| Poppy Education High School | Pape Clement | 1 Rue Léa Lagrange, 33650 Pessac, France | +33 5 57 26 03 00 | http://www.lyceepapecerme.fr |
| PERSEVERONS High School | Pré de Corlay | 4 Avenue Josephine Bales, 24200 Sarlat-la-Canéda, France | +33 5 55 31 70 70 | http://lyceepredecorlay-sarlat.com |
| Poppy Education High School | Raoul Follereau | 9 Boulevard Saint-Exupéry, 56000 Nantes, France | +33 3 86 30 36 00 | http://lyceefollereau.ac-dijon.fr |
| PERSEVERONS High School | René Cassin | 2 Rue de Lassus, 64100 Bayonne, France | +33 5 59 59 14 20 | http://webtab.ac-bordeaux.fr/lycee-renecassin |
| PERSEVERONS High School | Saint-Cricq | 4 Piste Cyclable, 64000 Pau, France | +33 5 59 59 72 01 | http://lycee-saint-cricq.org |
| PERSEVERONS High School | Saint-Genes | 160 Rue de Saint-Genes, 33000 Bordeaux, France | +33 5 56 33 84 34 | http://www.lyceesaintgenes.com |
| Poppy Education High School | Sainte-Mère-Église | 164 Rue François Mounier, 35220 Nantes, France | +33 5 59 38 02 13 | http://www.grandebrun.com |
| INRA | Sainte-Saintonge | 12 Rue de Saintonge, 33000 Bordeaux, France | +33 5 56 99 39 29 | http://www.lyceesaintlamine.com/ |
| Poppy Education High School | Victor Louis | 2 Rue de Mégret, 33400 Talence, France | +33 5 56 80 75 40 | http://lycee-victorlouis.fr |

**Figure 25. List of partner schools of the Poppy Education project**
The Arts and Métiers campus at Bordeaux-Talence in partnership with Inria contributes with its educational and scientific expertise to the development of new teaching methods and tools. The objective is to develop teaching sequences based on a project approach relying on an attractive multidisciplinary technological system: the humanoid Inria Poppy robot. These teaching sequences will be built and tailored to different levels of training, from high schools to Engineer schools.

The new formation "Bachelor of Technology", started in September 2014 at Ensam Bordeaux, is resolutely turned towards a project based pedagogy, outlining concepts from concrete situations. The humanoid Inria Poppy robot offers an open platform capable of providing an unifying thread for the different subjects covered during the 3-years of the Bachelor formation: mechanics, manufacturing (3D printing), electrical, mechatronics, computer sciences, design...

For the 1st and 2nd year of the ENSAM Engineer cursus, the Poppy robot is now used to support the teaching and to conduct further investigation.

9.1.3. KidLearn and Region Aquitaine

A Conseil Régional d’Aquitaine Project (KidLearn, 2015-) began, coordinated by Manuel Lopes entitled KidLearn. Will fund 50% of a 3 years PhD student.

We propose here a research project that aims at elaborating algorithms and software systems to help humans learn efficiently, at school, at home or at work, by adapting and personalizing sequences of learning activities to the particularities of each individual student. This project leverages recent innovative algorithmic models of human learning (curiosity in particular, developed as a result of ERC European project of the Flowers team), and combines it with state-of-the-art optimization algorithms and an original integration with existing expert knowledge (human teachers). Given a knowledge domain and a set of possible learning activities, it will be able to propose the right activity at the right time to maximize learning progress. It can be applied to many learning situations and potential users: children learning basic knowledge in schools and with the support of their teachers, older kids using educational software at home, of adults needing to acquire new skills through professional training (“formation professionnelle”). Because it combines innovations in computational sciences (machine learning and optimization) with theories of human cognition (theories of human learning and of education), this project is also implementing a strong cross-fertilization between technology and human sciences (SHS).

9.1.4. Comacina Capsule Creative Art/Science project and Idex/Univ. Bordeaux

The artist community is a rich source of inspiration and can provide new perspectives to scientific and technological questions. This complementarity is a great opportunity that we want to enforce in the Poppy project by making the robot accessible to non-robotic-expert users. The Comacina project, in collaboration with the Flowers team and supported by funding from Idex/Univ. Bordeaux, explored the role of movements and light in expressing emotions: http://comacina.org . This project was implemented through several residencies during the year, and several performances at various cultural places in Aquitaine, including at Pole Evasion in Ambares-et-Lagra
de. a report is available at https://flowers.inria.fr/RencontreAutourDuGeste.pdf . It benefitted from funding from the Art/Science Idex call for project.

9.2. National Initiatives

PY Oudeyer collaborated with Aymar de Rugy, Daniel Cattaert, Mathilde Couraud, Sébastien Mick and Florent Paclet (INCIA, CNRS/Univ. Bordeaux) about the design of myoelectric robotic prostheses based on the Poppy platform, and on the design of algorithms for co-adaptation learning between the human user and the prosthesis. This was funded by a PEPS CNRS grant.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. 3rd HAND

Title: Semi-Autonomous 3rd Hand
Programm: FP7
Duration: October 2013 - September 2017
Coordinator: Inria
Partners:
- Technische Universität Darmstadt (Germany)
- Universität Innsbruck (Austria)
- Universität Stuttgart (Germany)
Inria contact: Manuel Lopes

Robots have been essential for keeping industrial manufacturing in Europe. Most factories have large numbers of robots in a fixed setup and few programs that produce the exact same product hundreds of thousands times. The only common interaction between the robot and the human worker has become the so-called ‘emergency stop button’. As a result, re-programming robots for new or personalized products has become a key bottleneck for keeping manufacturing jobs in Europe. The core requirement to date has been the production in large numbers or at a high price. Robot-based small series production requires a major breakthrough in robotics: the development of a new class of semi-autonomous robots that can decrease this cost substantially. Such robots need to be aware of the human worker, alleviating him from the monotonous repetitive tasks while keeping him in the loop where his intelligence makes a substantial difference. In this project, we pursue this breakthrough by developing a semi-autonomous robot assistant that acts as a third hand of a human worker. It will be straightforward to instruct even by an untrained layman worker, allow for efficient knowledge transfer between tasks and enable a effective collaboration between a human worker with a robot third hand. The main contributions of this project will be the scientific principles of semi-autonomous human-robot collaboration, a new semi-autonomous robotic system that is able to: i) learn cooperative tasks from demonstration; ii) learn from instruction; and iii) transfer knowledge between tasks and environments. We will demonstrate its efficiency in the collaborative assembly of an IKEA-like shelf where the robot acts as a semiautonomous 3rd-Hand.

9.3.1.2. DREAM

Title: Deferred Restructuring of Experience in Autonomous Machines
Programm: H2020
Duration: January 2015 - December 2018
Coordinator: UPMC
Partners:
- Armines (ENSTA ParisTech)
- Queen Mary University London (England)
- University of A Coruna (Spain)
- Vrije University Amsterdam (Holland)
Contact: David Filliat

Abstract: A holy grail in robotics and artificial intelligence is to design a machine that can accumulate adaptations on developmental time scales of months and years. From infancy through adulthood, such a system must continually consolidate and bootstrap its knowledge, to ensure that the learned knowledge and skills are compositional, and organized into meaningful hierarchies. Consolidation of previous experience and knowledge appears to be one of the main purposes of sleep and dreams for humans, that serve to tidy the brain by removing excess information, to recombine concepts to improve information processing, and to consolidate memory. Our approach – Deferred Restructuring of Experience in Autonomous Machines (DREAM) – incorporates sleep and dream-like processes within a cognitive architecture. This enables an individual robot or groups of robots to consolidate their experience into more useful and generic formats, thus improving their future ability to learn and adapt. DREAM relies on Evolutionary Neurodynamic ensemble methods (Fernando et al, 2012 Frontiers in Comp Neuro; Bellas et al., IEEE-TAMD, 2010 ) as a unifying principle for discovery, optimization, re-structuring and consolidation of knowledge. This new paradigm will make the robot more autonomous in its acquisition, organization and use of knowledge and skills just as long as they comply with the satisfaction of pre-established basic motivations. DREAM will enable robots to cope with the complexity of being an information-processing entity in domains that are open-ended both in terms of space and time. It paves the way for a new generation of robots whose existence and purpose goes far beyond the mere execution of dull tasks. http://www.robotsthatdream.eu

9.3.2. Collaborations in European Programs, except FP7 & H2020

9.3.2.1. IGLU

Title: Interactive Grounded Language Understanding (IGLU)
Program: CHIST-ERA
Duration: October 2015 - September 2018
Coordinator: University of Sherbrooke, Canada
Partners:
- University of Sherbrooke, Canada
- Inria Bordeaux, France
- University of Mons, Belgium
- KTH Royal Institute of Technology, Sweden
- University of Zaragoza, Spain
- University of Lille 1, France
- University of Montreal, Canada

Inria contact: Pierre-Yves Oudeyer

Language is an ability that develops in young children through joint interaction with their caretakers and their physical environment. At this level, human language understanding could be referred as interpreting and expressing semantic concepts (e.g. objects, actions and relations) through what can be perceived (or inferred) from current context in the environment. Previous work in the field of artificial intelligence has failed to address the acquisition of such perceptually-grounded knowledge in virtual agents (avatars), mainly because of the lack of physical embodiment (ability to interact physically) and dialogue, communication skills (ability to interact verbally). We believe that robotic agents are more appropriate for this task, and that interaction is a so important aspect of human language learning and understanding that pragmatic knowledge (identifying or conveying intention) must be present to complement semantic knowledge. Through a developmental approach where knowledge grows in complexity while driven by multimodal experience and language interaction with a human, we propose an agent that will incorporate models of dialogues, human emotions and intentions as part of its decision-making process. This will lead anticipation and reaction not only
based on its internal state (own goal and intention, perception of the environment), but also on the perceived state and intention of the human interactant. This will be possible through the development of advanced machine learning methods (combining developmental, deep and reinforcement learning) to handle large-scale multimodal inputs, besides leveraging state-of-the-art technological components involved in a language-based dialog system available within the consortium. Evaluations of learned skills and knowledge will be performed using an integrated architecture in a culinary use-case, and novel databases enabling research in grounded human language understanding will be released. IGLU will gather an interdisciplinary consortium composed of committed and experienced researchers in machine learning, neurosciences and cognitive sciences, developmental robotics, speech and language technologies, and multimodal/multimedia signal processing. We expect to have key impacts in the development of more interactive and adaptable systems sharing our environment in everyday life. http://iglu-chistera.github.io/

9.4. International Initiatives

9.4.1. Inria Associate Teams Not Involved in an Inria International Labs

9.4.1.1. NEUROCURIOSITY

Title: NeuroCuriosity

International Partner (Institution - Laboratory - Researcher):

Columbia Neuroscience (United States) - Cognitive Neuroscience - JACQUELINE GOTTLIEB

Start year: 2016

See also: https://flowers.inria.fr/neurocuriosity

Curiosity can be understood as a family of mechanisms that evolved to allow agents to maximize their knowledge of the useful properties of the world. In this project we will study how different internal drives of an animal, e.g. for novelty, for action, for liking, are combined to generate the rich variety of behaviors found in nature. We will approach such challenge by studying monkeys, children and by developing new computational tools.

9.4.1.2. Informal International Partners

Pierre-Yves Oudeyer and Didier Roy have create a collaboration with LSRO EPFL and Pr Francesco Mondada, about Robotics and education. The two teams co-organize the annual conference "Robotics and Education" in Bordeaux. Didier Roy teaches "Robotics and Education" in EPFL several times a year.

Pierre-Yves Oudeyer collaborated with Edith Law’s HCI research group at University of Waterloo on the topic of "Curiosity in HCI system". They co-organized the "Designing for curiosity" workshop at CHI 2017, Denver, Colorado, and obtained a grant from Univ. Bordeaux to set up a project with Inria Potioc team and with Dana Kulic, Robotics lab, Univ. Waterloo.

Didier Roy has created a collaboration with HEP VAud (Teachers High School) and Bernard Baumberger and Morgane Chevalier, about Robotics and education. Scientific discussions and shared professional training.

Florian Golemo is in an active collaboration with Aaron Courville from MILA Montreal to work on the IGLU project together.

William Schueller visited Vittorio Loreto’s team in Rome from January till August 2017, funded by the Idex program of the University of Bordeaux. Vittorio Loreto is an Associate Professor in Physics at University Sapienza of Rome, and head of the research team Social Dynamics Lab. William Schueller also participated to a conference organized by V. Loreto in Rome, the Kreyon Conference, by giving a talk and presenting a user experiment: an interactive Naming Game.
9.4.2. Participation in Other International Programs

David Filliat participates in the ITEA3 DANGUN project with Renault S.A.S. in France and partners in Korea. The purpose of the DANGUN project is to develop a Traffic Jam Pilot function with autonomous capabilities using low-cost automotive components operating in France and Korea. By incorporating low-cost advanced sensors and simplifying the vehicle designs as well as testing in different scenarios (France & Korea), a solution that is the result of technical cooperation between both countries should lead to more affordable propositions to respond to client needs in the fast moving market of intelligent mobility.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Georges Kachergis, University of Radboud, The Netherlands
- Cynthia Liem, University of Delft, The Netherlands
- Mike Schaerkermann, Univ. Waterloo, Canada
- Roboy team, University of Munich, Germany
- Lauriane Rat-Fiseher, Univ. Toulouse, France
- Mai Nguyen, ENST Bretagne, France

9.5.1.1. Internships

- Kelian Schindowski, project Poppy Education
- Octave Delorme, project Poppy Education
- Alexandre Péré, Deep learning and intrinsic motivation
- Pierre Manceron, Deep Reinforcement Learning
- Timothée Anne, Intrinsically Motivated Goal Exploration

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- PY. Oudeyer has been general co-chair of the "Designing for curiosity" workshop at CHI 2017, Denver, Colorado, US;
- PY. Oudeyer has co-organized the 3rd International Symposium on Intrinsically Motivated Open-Ended Learning, Rome, Italy;
- PY. Oudeyer has co-organized the IEEE IJCNN 2017 Special Session on COGNITION AND DEVELOPMENT;
- D. Roy was general chair for the conference "Robotique et Education", Bordeaux, France.

10.1.1.2. Member of the Organizing Committees

- PY. Oudeyer has been "Robotics Liaison" of IJCNN 2017, Anchorage, Alaska.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

- PY. Oudeyer has been in the conference program committee of IEEE ICDL-Epirob conference.

10.1.2.2. Reviewer
• David Filliat was reviewer for the IROS, ECMR, ICDL, HRI, ICRA conferences.
• Sébastien Forestier was reviewer for IEEE ICDL-Epirob, ICRA
• Natalia Díaz Rodríguez was reviewer for JAIR 2017 (Journal of AI Research) and Area Chair (meta-reviewer) for WIML 2017 (Women in Machine Learning Workshops at NIPS 2017).

10.1.3. Journal
10.1.3.1. Member of the Editorial Boards
• PY. Oudeyer was associate editor of IEEE Transactions on CDS and Frontiers in Neurorobotics.

10.1.3.2. Reviewer - Reviewing Activities
• O. Sigaud has been a reviewer for the Autonomous Robots journal and for the ICLR and the NIPS conferences
• PY. Oudeyer has been a reviewer for the journals IEEE Transactions on CDS and Child and Development Perspectives.

10.1.4. Invited Talks
• David Filliat gave an invited presentation “Autonomous Learning and AI for interactive Robotics” during the 50 years of Inria event on November 8th.
• O. Sigaud gave an invited presentation “Deep Learning for Robotics: Promises and Issues” at the Journées Nationales de la Recherche en Robotique on November 16th.
• O. Sigaud gave an invited presentation “Towards developmental discovery of objects in dynamical scenes” at the workshop on Intrinsically Motivated Open-Ended Learning, Rome, Italy, 9th October
• PY. Oudeyer gave an invited presentation "Intrinsically Motivated Goal Exploration Processes” at the workshop on Intrinsically Motivated Open-Ended Learning, Rome, Italy, 9th October;
• PY. Oudeyer gave an invited presentation "Computational Models of Human Cognitive Development” at the 29th Eleanor Gibson lecture, Cornell Univ., US, April,
• PY. Oudeyer gave an invited presentation "Models of curiosity-driven learning” at Univ. Rochester, US, April.
• PY. Oudeyer gave an invited presentation "Curiosity-driven learning and language acquisition” at the workshop on language acquisition at IEEE ICDL-Epirob, Lisbon, Portugal, Sept.;
• PY. Oudeyer gave an invited presentation "Robotique Pédagogique” at the Journées Nationales de la Recherche en Robotique on November 16th.
• PY. Oudeyer gave an invited presentation "Intrinsically motivated learning and curiosity in humans and robots" at the "Designing for curiosity" workshop at CHI 2017, Denver, US;

10.1.5. Leadership within the Scientific Community
• Natalia Díaz Rodríguez attended and organized a workshop within the Heidelberg Laureate Forum Sept. 2017 on Machine learning and Human-Computer Interaction.
• PY. Oudeyer co-organized the "Designing for curiosity” workshop at CHI 2017 (Denver, US), the IMOL 2017 workshop (Rome, Italy), and was co-editor of the special issue on "Modeling play in early infant development” in Frontiers in Psychology.
• PY. Oudeyer has been editor of the IEEE CIS Newsletter on Cognitive and Developmental systems, organizing two interdisciplinary dialogs, see https://openlab-flowers.inria.fr/t/ieee-cis-newsletter-on-cognitive-and-developmental-systems/129.

10.1.6. Scientific Expertise
• PY. Oudeyer has been a reviewer for the European Commission (FET program).
10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master: Robotique Mobile, 21 heures. M2, ENSTA - ParisTech (David Filliat).
Master: Perception pour la Robotique, 6 heures. M2, ENSTA - ParisTech (David Filliat).
Master: Perception pour la robotique, 12 heures. M2 Systemes Avances et Robotique, University Pierre et Marie Curie (David Filliat)
Master: Perception pour la Robotique Développementale, 3 hours, CogMaster (David Filliat)
Licence Informatique, 64h Bordeaux University (Sébastien Forestier)
Master: Perception pour les systemes autonomes (ROB313), 7.50 h. Natalia Díaz Rodríguez
Master: Projet Informatique (IN104), 18.25h. Natalia Díaz Rodríguez.
Master: Cours de robotique développementale, option robot, ENSEIRB (2h), PY. Oudeyer

10.2.2. Supervision

PhD in progress: Cédric Colas, Algorithms for intrinsically motivated goal exploration (superv. P-Y. Oudeyer)
PhD in progress: Sébastien Forestier, Models of curiosity-driven learning of tool use and speech development, started in sept. 2015 (superv. P-Y. Oudeyer)
PhD in progress: William Schueller, Study of the impact of active learning and teaching in naming games dynamics, started in sept. 2015 (superv. P-Y. Oudeyer)
PhD in progress: Thibault Desprez, Design and study of the impact of educational robotic kits in computer science education, started in dec. 2016 (superv. P-Y. Oudeyer)
PY. Oudeyer supervised a team of computer and pedagogical engineers and researchers for the project Poppy Education (Didier Roy, Stéphanie Noirpoudre, Théo Segonds, Damien Caselli)
PhD: Thibaut Munzer, Learning from Instruction, defended (superv. Manuel Lopes).
PhD in progress: Baptiste Busch, Interactive Learning, started oct 2014 (superv. Manuel Lopes).
PhD: Yuxin Chen, Interactive learning of objects and names on a humanoid robot, defended 02/2017 (superv. David Filliat).
PhD: Celine Craye, Curiosity and visual attention for the guidance of an exploration robot, defended 04/2017 (superv. David Filliat).
PhD: Joris Guery, Robust visual recognition by artificial neural networks in robotic exploration scenarios, defended 11/2017 (superv. David Filliat and Bertrand Le Saulx (ONERA))
PhD in progress: Adrien Matricon : Task dependent visual feature selection for optimising and generalizing robotics skills (superv. David Filliat, Pierre-Yves Oudeyer).
PhD in progress: José Magno Mendes Filho, Planning and control of an autonomous AGV in environment shared with humans, started Oct. 2015 (superv. David Filliat and Eric Lucet (CEA))
PhD in progress: Timothée Lesort, Incremental Deep Learning for Detection and Classification in a Robotic Context. started june 2017 (superv. David Filliat and Jean-Francois Goudou (THALES)).
PhD in progress: Vyshakh Palli Thazha, Data fusion for autonomous vehicles. started sept 2017 (superv. David Filliat and Hervé Illy (Renault)).

10.2.3. Juries
David Filliat was in the jury of Houssem Nouira (20/04/2017, Examinateur) : Affinement de relevés laser mobiles issus de Lidars multi-couches
David Filliat was in the jury of Quan Nguyen (06/10/2017, Rapporteur) : Mapping of a sound environment by a mobile robot
David Filliat was in the jury of Vijaya kumar Ghorpade (20/12/2017, Examinateur) : 3D Semantic mapping for indoor navigation
PY. Oudeyer was in the PhD juries of Céline Craye (ENSTA), Gabriel Sulem (ENS), Arthur Prat-Carrabin (ENS), Miquel Cornudella (ENS)
PY. Oudeyer was in the HdR jury of Alexandre Pitti (Univ. Cergy Pontoise)

10.3. Popularization

10.3.1. Duties

D. Roy is member of the Class’code team (Inria is member of the consortium of this project) https://pixees.fr/classcode/accueil/. Class’code is a blended formation for teachers and animators who aim to initiate young people to computer science and robotics. D. Roy has in charge the robotics module of the project.
D. Roy is adviser of the organization of computer science exhibition in "Palais de la découverte" which will begin on 2018 March. He helps for robotics part.
D. Roy is member of the team "Education en Scène" which organize educational activities with robotics in Bordeaux Digital City.
D. Roy is member of the scientific committee of "Didapro Didastic" Conference which will be held in Lausanne (Switzerland) on 2018 February.
D. Roy is member of the Robocup Junior French committee, an international robotics challenge http://rcj.robocup.org/.
D. Roy is member of the scientific committee of "Ludovia CH" Conference which will be held in Yverdon (Switzerland) on 2018 March.
D. Roy is project leader of Thymio Simulator for Classcode project. Specifications and coordination of work.
D. Roy is project leader of Thymio Scratch and Thymio Snap! development, with D. Sherman. Inria, EPFL and Mobsya collaboration.
PY. Oudeyer continued to be the PI of the Poppy Education project.

10.3.2. Online content

Stephanie Noirpoudre. Atelier Poppy Ergo Jr au CERN. Description and feedback of a workshop on the construction and programming of the robotic arm Poppy Ergo Jr as part of the Coding Pi Science Event. [83]
Stephanie Noirpoudre. Robotic workshop at CERN. Description and feedback of a workshop on the construction and programming of the robotic arm Poppy Ergo Jr as part of the Coding Pi Science Event. [84]
Stephanie Noirpoudre, Kélian Schindowsky. Poppy Education présent à la journée EIDOS 64 : Le forum des pratiques numériques pour l'éducation. Description and feedback of the 9th edition of the EIDOS64 day (the digital practice forum for education). [85]
Sylvain Soulard, Kélian Schindowsky. Description of activity "Modeling of the Port of Rotterdam" using the robot arm Poppy Ergo Jr and created by Sylvain Soulard, middle school teacher in technology. He started the problem: how to optimize and secure the transport of containers in a commercial port? [88]
Kelian Schindowsky. Un projet étudiant : des mains pour Poppy Torso ! Utilisation de la plateforme Poppy pour un projet étudiant. A use of the Poppy platform for a student project: 4 Poppy Torso robots modified by the students of the Bordeaux-Talence campus clashed in the large amphitheater. A competition of a new kind including free figures and imposed figures. [87]

Kelian Schindowsky. Des roues pour le robot Poppy Torso : New Bachelor of Technology students from ENSAM (Talence) worked on the Poppy Torso robot, the goal this time was to equip it with a mobile platform. [86]

10.3.3. Teaching and Education

10.3.3.1. Poppy Education

January 2017, meeting with partner teachers
March 2017, meeting with partner teachers
March 2017, training day with new teachers partners - Building and programming the robot Poppy Ergo Jr
May 2017, meeting with partner teachers
September 2017, meeting with partner teachers
June 2017, training day with workers from Cap’Metier and Cultures électroniques (for scientific mediation purpose) to initiate to robotic - Building and programming the robot Poppy Ergo Jr

10.3.3.2. Inirobot

May 2017, Plan national de formation organised by La main à la pâte (Paris): D. ROY - Train future trainers to inirobot curriculum
April 2017, Training days organized by Main à la pâte for National Education (CEA Saclay): T. Desprez, S. Noirpoudre, D. Roy, Théo Segonds - Train a group of teachers to inirobot

10.3.4. Talks and Hands-on

10.3.4.1. KidBreath


10.3.4.2. Poppy Education

January 2017, Eidos64 event - Le forum des pratiques numériques pour l’éducation (Lons): S. Noirpoudre, K. Schindowsky - Talk to present Poppy Education
Janvier 2017, Visit organized by Le Conseil Départemental des Jeunes (Inria Bordeaux Sud-Ouest): S. Noirpoudre - Programming workshops (for middle school students) to initiate in programmation with Poppy Ergo Jr robot
January 2017, Robotics training day organised by Maison pour la Science (Inria Bordeaux Sud-Ouest): S. Noirpoudre, T. Desprez - Programming workshop (for futur trainers) to initiate in programmation with Poppy Ergo Jr robot
January 2017, R2T2 AmeriCarabeaen (island of Martinique) : D. Roy - Co-organization with EPFL and ESPE of Martinique - International event (Mexico, Quebec, Guyane, Sainte Lucie) about robotics for education http://www.reseau-espe.fr/actualites/espe-de-martinique-le-defi-r2t2-americaraibe-ete-releve
March 2017, Education exhibition Eduspot (Paris): S. Noirpoudre - Exhibition stand to present the robotic platform Poppy and the use in Education
March 2017, Le printemps de la mixité event (Inria Bordeaux Sud-Ouest): S. Noirpoudre - Robotics workshops (for high school students) to initiate in programmation with Poppy Ergo Jr robot
April 2017, Training days organized by Main à la pâte for National Education (CEA Saclay): T. Desprez, S. Noirpoudre, D. Roy, Théo Segonds - Train a group of teachers to robotics and programmation with Poppy Ergo Jr robot

May 2017, Plan national de formation organised by La main à la pâte (Paris): S. Noirpoudre - Talk to present Poppy Education project and Poppy Ergo Jr


May 2017, Robot makers’day (Talence): K. Schindowsky - Exhibition stand to present Poppy Education and Poppy robots

May 2017, RII Santiago (Santiago de Chile, Chile): T. Segonds - Exhibition stand to present Poppy Education and Poppy robots - Event organized by Inria Chile

May 2017, Bordeaux Geek Festival (Bordeaux): K. Schindowsky - Workshops to initiate in programming

May 2017, PY. Oudeyer gave an invited presentation on “Robotics and cognitive sciences” at Festival Filosofia, St. Emilion, France

June 2017, Internships: observation Sequence for Grade 3 Students (Inria Bordeaux Sud-Ouest - Welcome two students from middle-school during a week to discover the working environment and to introduce them to robotics

June 2017, Robotics workshop for a primary class (Inria Bordeaux Sud-Ouest): S. Noirpoudre, T. Desprez - Poppy Education and inirobot workshops

June 2017, EIAH : Environnements informatiques pour l’apprentissage humain (Strasbourg): S. Noirpoudre, T. Desprez - Talk to present the article “Poppy Education : un dispositif robotique open source pour l’enseignement de l’informatique et de la robotique”

June 2017, EIAH : Environnements informatiques pour l’apprentissage humain (Strasbourg): T. Desprez, S. Noirpoudre - Exhibition stand to present the robotics platform Poppy and the use in Education

June 2017, Rencontre avenir numérique alsace (strasbourg): S. Noirpoudre - Talk in videoconference to present Poppy Education and the robot Poppy Ergo Jr


July 2017, Symposium Education and Robotics (Bordeaux): D. Roy (coordinator) and Flowers Team Members - Organization of the colloquium

July 2017, Symposium Education and Robotics (Bordeaux): S. Noirpoudre - Talk to present Poppy Education project

July 2017, Symposium Education and Robotics (Bordeaux): PY. Oudeyer - Talk to present Flowers educational robotics projects

July 2017, Symposium Education and Robotics (Bordeaux): S. Noirpoudre - Exhibition stand to present the robotics platform Poppy and the use in Education

July 2017, 10th International Scratch conference (Bordeaux): D. Roy - Member of the Scratch organizing committee, member of the scientific committee - the conference organization begun on december 2017

July 2017, 10th International Scratch conference (Bordeaux): T. Segonds - Talk to present Poppy Education project
July 2017, 10th International Scratch conference (Bordeaux): S. Noirpoudre - Exhibition stand to present the robotics platform Poppy and the use in Education
August 2017, Fab13 Fabricating Society Conference (Santiago de Chile, Chile): T. Segonds - Talk on Poppy Education - Two days workshop on using and modifying Poppy robots
October 2017, Coding Pi Science Days (CERN and Hepia engineering school at Geneva): T. Segonds, T. Desprez - Talk to present the robotics platform Poppy and the use in Education - Three days robotics workshops on building and programming a Poppy Ergo Jr robot
October 2017, Fête de la science (Inria Bordeaux Sud-Ouest): D. Roy - special event with a robotics workshop and several demos at Inria Center, with members of staff of Bordeaux Metropole and political actors
October 2017, Fête de la science (Inria Bordeaux Sud-Ouest): T. Segonds, T. Desprez - 8 programming workshop in 2 days (with middle school students) using Snap! and the robot Poppy Ergo Jr
November 2017, JNRR (National Days of Robotics Research, Biarritz): D. Roy (moderator), P.-Y. Oudeyer (speaker) - Talk on Educational Robotics -
December 2017, Aperobot Bordeaux (Bordeaux): T. Segonds - Poppy Ergo Jr programming workshop
December 2017, Internships: observation Sequence for Grade 3 Students (Inria Bordeaux Sud-Ouest) - Welcomed three students from middle-school during a week to discover the working environment and to introduce them to robotics

10.3.5. Popularizing inside Inria

- March 2017, training day with Inria workers from scientific mediation - Building and programming the robot Poppy Ergo Jr
- October 2017, DevDays (Inria Bordeaux Sud-Ouest): D. Caselli - Presentation of the hotspot tool used in Poppy Ergo Jr robot

10.3.6. Creation of Material for Popularization

As part of the Poppy Education project, thanks the robotic platform Poppy we created pedagogical kits open-source and low cost for teaching computer science and robotics. It is designed to help young people to take ownership with concepts and technologies of the digital world.

The Pedagogical kits includes robots and pedagogical resources. They have been co-created directly with users (mainly high schools teachers) and evaluated in real life by experiments in classrooms [81]. The activities were designed with the visual programming language Snap! (Scratch like) and Python, but some are in Java / Processing (thanks the robot API you can use the language of your choice).
Most activities are using the robot Poppy Ergo Jr, but some use Poppy Torso (mostly in higher school because of its cost) and Poppy Humanoid (in kindergarten for dance projects):

- The Poppy Ergo Jr robot is a small and low cost 6-degree-of-freedom robot arm. It consists of simple shapes which can be easily 3D printed. It has several 3D printed tools extending its capabilities (there are currently the lampshade, the gripper and a pen holder but you can design new ones). They are assembled via rivets which can be removed and added very quickly with the OLLO tool. Each motor has LEDs on (8 different color can be activated). The electronic card (raspberry Pi) is visible next to the robot, that allow to manipulate, and plug extra sensors.

- The Poppy Torso robot is an open-source humanoid robot torso which can be installed easily on tabletops. More affordable than the robot Poppy Humanoid, it is an ideal medium to learn science, technology, engineering and mathematics.

We continued to improve the robots functionalities and you can see below the resources we created:

- A website have been created to present the project and to share all resources and activities: [https://www.poppy-education.org/](https://www.poppy-education.org/)

- To complete the pedagogical booklet [48] that provides guided activities and small challenges to become familiar with Poppy Ergo Jr robot and the Programming language Snap! ([https://drive.google.com/file/d/0B2jV8VX-lQHwTUxXZjF3OGxHVGM/view](https://drive.google.com/file/d/0B2jV8VX-lQHwTUxXZjF3OGxHVGM/view)) we provided a list of Education projects. Educational projects have been written for each activity carried out and tested in class. So each projects have its own web page including resources allowing any other teacher to carry out the activity (description, pedagogical sheet, photos/videos, pupil’s sheet, teacher’s sheet with correction etc.). Their is now 32 activities documented available on Poppy Education website.

You can see the activities on this links (in french):


- Primary Schools level : [https://www.poppy-education.org/activites/activites-primaire/](https://www.poppy-education.org/activites/activites-primaire/)

- Demonstrations (just videos to show the possibilities) : [https://www.poppy-education.org/activites/demos/](https://www.poppy-education.org/activites/demos/)

- We continued to improve the documentation of the robotic platform Poppy ([https://docs.poppy-project.org/en/](https://docs.poppy-project.org/en/)) and the documentation has been translated into French ([https://docs.poppy-project.org/fr/](https://docs.poppy-project.org/fr/)).

- A FAQ have been written with the most frequents questions to help users: [https://www.poppy-education.org/aide/](https://www.poppy-education.org/aide/)
10.3.7. Innovation and transfer

- Since 1 September 2017 until February 2019, PerPoppy and Poppy Station Projects: D. Roy, P.-Y. Oudeyer. These projects aim to perpetuate the Poppy robot ecosystem by creating an external structure from outside Inria, with various partners. After the Poppy Robot Project, the Poppy Education Project is ending and Inria doesn’t.

Many exchanges have already taken place with potential partners such as the EPFL, the ENSAM network, the «Ligue de l’Enseignement», Génération Robots, the French Institute of Education, several academies, the direction of digital education of the Ministry of Education, ... PerPoppy is the project which is building the new structure, and Poppy Station is the new name of the new structure. Poppy Station, which will include Poppy robot ecosystem (hardware, software, community) from the beginning, will be a place of excellence to build future educational robots and to design pedagogical activities to teach computer science, robotics and Artificial Intelligence.

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**Publications of the year**

**Articles in International Peer-Reviewed Journal**


**International Conferences with Proceedings**


**Conferences without Proceedings**


**Scientific Popularization**

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**Other Publications**


**References in notes**


Project-Team GEOSTAT

Geometry and Statistics in acquisition data

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Optimization, machine learning and statistical methods
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Project-Team GEOSTAT

Creation of the Team: 2009 November 01, updated into Project-Team: 2011 January 01

Keywords:

Computer Science and Digital Science:
A3.4.2. - Unsupervised learning
A3.4.7. - Kernel methods
A3.4.8. - Deep learning
A5.3. - Image processing and analysis
A5.3.2. - Sparse modeling and image representation
A5.3.3. - Pattern recognition
A5.3.5. - Computational photography
A5.7. - Audio modeling and processing
A5.7.3. - Speech
A5.7.4. - Analysis
A5.9. - Signal processing
A5.9.2. - Estimation, modeling
A5.9.3. - Reconstruction, enhancement
A5.9.5. - Sparsity-aware processing

Other Research Topics and Application Domains:
B2. - Health
B2.2. - Physiology and diseases
B2.2.1. - Cardiovascular and respiratory diseases
B2.2.6. - Neurodegenerative diseases
B3. - Environment and planet
B3.3. - Geosciences
B3.3.2. - Water: sea & ocean, lake & river
B3.3.4. - Atmosphere

1. Personnel

Research Scientists
Hussein Yahia [Team leader, Inria, Researcher, HDR]
Khalid Daoudi [Inria, Researcher]
Nicolas Brodu [Inria, Researcher]
Guillaume Attuel [Inria, Starting Research Position, from Mar 2017]

Technical Staff
Marie Martin [Inria, from Jul 2017]

PhD Students
Anass El Aouni [Inria, Univ Rabat]
Camila Artana [Univ Pierre et Marie Curie]
Gopal Singh [Indian Institute of Technology Roorkee]

Post-Doctoral Fellow
2. Overall Objectives

2.1. Overall Objectives

GEOSTAT is a research project which investigates the analysis of some classes of natural complex signals (physiological time series, turbulent universe and earth observation data sets) by determining, in acquired signals, the properties that are predicted by commonly admitted or new physical models best fitting the phenomenon. Consequently, when statistical properties discovered in the signals do not match closely enough those predicted by accepted physical models, we question the validity of existing models or propose, whenever possible, modifications or extensions of existing models. We will give, in the sequel, a detailed example of this approach and methodology (Heart electrical activity signal analysis). An important aspect of this methodological approach is that we don’t rely in GEOSTAT, on a predetermined “universal” signal processing model to analyze natural complex signals. Instead, we take into consideration existing approaches in nonlinear signal processing (wavelets, multifractal analysis tools such as log-cumulants or micro-canonical multifractal formalism, time frequency analysis etc.) which are used to determine the micro structures or other micro features inside the acquired signals. Then, statistical analysis of these micro data are determined and compared to expected behaviour from theoretical physical models used to describe the phenomenon from which the data is acquired. From there different possibilities can be contemplated:

- The statistics match behaviour predicted by the model: complexity parameters predicted by the model are extracted from signals to analyze the dynamics of underlying phenomena. Examples: analysis of turbulent data sets in Oceanography and Astronomy.

- The signals displays statistics that cannot be attainable by the common lore of accepted models: how to extend or modify the models according to the behaviour of observed signals? Example: electrical activity of heart signal analysis (see infra).

GEOSTAT is a research project in nonlinear signal processing which develops on these considerations: it considers the signals as the realizations of complex extended dynamical systems. The driving approach is to describe the relations between complexity (or information content) and the geometric organization of information in a signal. For instance, for signals which are acquisitions of turbulent fluids, the organization of information may be related to the effective presence of a multiscale hierarchy of coherent structures, of multifractal nature, which is strongly related to intermittency and multiplicative cascade phenomena; the determination of this geometric organization unlocks key nonlinear parameters and features associated to these signals; it helps understand their dynamical properties and their analysis. We use this approach to derive novel solution methods for super-resolution and data fusion in Universe Sciences acquisitions [10].

Another example can be found in signal analysis of the electrical activity of the heart, where we find the distribution of activation points in a signal during episodes of atrial fibrilation (with strengthening from feature selection and Bayesian learning see below). Specific advances are obtained in GEOSTAT in using this type of statistical/geometric approach to get validated dynamical information of signals acquired in Universe Sciences, e.g. Oceanography or Astronomy. The research in GEOSTAT encompasses nonlinear signal processing and the study of emergence in complex systems, with a strong emphasis on geometric approaches to complexity. Consequently, research in GEOSTAT is oriented towards the determination, in real signals, of quantities or
phenomena, usually unattainable through linear methods, that are known to play an important role both in the evolution of dynamical systems whose acquisitions are the signals under study, and in the compact representations of the signals themselves.

Signals studied in GEOSTAT belong to two broad classes:

- Acquisitions in Astronomy and Earth Observation.
- Physiological time series.

### 3. Research Program

#### 3.1. General methodology

- **Fully Developed Turbulence (FDT)** Turbulence at very high Reynolds numbers; systems in FDT are beyond deterministic chaos, and symmetries are restored in a statistical sense only, and multi-scale correlated structures are landmarks. Generalizing to more random uncorrelated multi-scale structured turbulent fields.

- **Compact Representation** Reduced representation of a complex signal (dimensionality reduction) from which the whole signal can be reconstructed. The reduced representation can correspond to points randomly chosen, such as in Compressive Sensing, or to geometric localization related to statistical information content (framework of reconstructible systems).

- **Sparse representation** The representation of a signal as a linear combination of elements taken in a dictionary (frame or basis), with the aim of finding as less as possible non-zero coefficients for a large class of signals.

- **Universality class** In theoretical physics, the observation of the coincidence of the critical exponents (behaviour near a second order phase transition) in different phenomena and systems is called universality. Universality is explained by the theory of the renormalization group, allowing for the determination of the changes followed by structured fluctuations under rescaling, a physical system is the stage of. The notion is applicable with caution and some differences to generalized out-of-equilibrium or disordered systems. Non-universal exponents (without definite classes) exist in some universal slowing dynamical phenomena like the glass transition and kindred. As a consequence, different macroscopic phenomena displaying multiscale structures (and their acquisition in the form of complex signals) may be grouped into different sets of generalized classes.

Every signal conveys, as a measure experiment, information on the physical system whose signal is an acquisition of. As a consequence, it seems natural that signal analysis or compression should make use of physical modelling of phenomena: the goal is to find new methodologies in signal processing that goes beyond the simple problem of interpretation. Physics of disordered systems, and specifically physics of (spin) glasses is putting forward new algorithmic resolution methods in various domains such as optimization, compressive sensing etc. with significant success notably for NP hard problem heuristics. Similarly, physics of turbulence introduces phenomenological approaches involving multifractality. Energy cascades are indeed closely related to geometrical manifolds defined through random processes. At these structures’ scales, information in the process is lost by dissipation (close to the lower bound of inertial range). However, all the cascade is encoded in the geometric manifolds, through long or short distance correlations depending on cases. How do these geometrical manifold structures organize in space and time, in other words, how does the scale entropy cascades itself ? To unify these two notions, a description in term of free energy of a generic physical model is sometimes possible, such as an elastic interface model in a random nonlinear energy landscape : This is for instance the correspondence between compressible stochastic Burgers equation and directed polymers in a disordered medium. Thus, trying to unlock the fingerprints of cascade-like structures in acquired natural signals becomes a fundamental problem, from both theoretical and applicative viewpoints.
To illustrate the general methodology undertaken, let us focus on an example conducted in the study of physiological time series: the analysis of signals recorded from the electrical activity of the heart in the general setting of Atrial Fibrillation (AF). AF is a cardiac arrhythmia characterized by rapid and irregular atrial electrical activity with a high clinical impact on stroke incidence. Best available therapeutic strategies combine pharmacological and surgical means. But when successful, they do not always prevent long-term relapses. Initial success becomes all the more tricky to achieve as the arrhythmia maintains itself and the pathology evolves into sustained or chronic AF. This raises the open crucial issue of deciphering the mechanisms that govern the onset of AF as well as its perpetuation. We have developed a wavelet-based multi-scale strategy to analyze the electrical activity of human hearts recorded by catheter electrodes, positioned in the coronary sinus (CS), during episodes of chronic AF. We have computed the so-called multifractal spectra using two variants of the wavelet transform modulus maxima method, the moment (partition function) method and the magnitude cumulant method (checking confidence intervals with surrogate data). Application of these methods to long time series recorded in a patient with chronic AF provides quantitative evidence of the multifractal intermittent nature of the electric energy of passing cardiac impulses at low frequencies, i.e. for times ($\gtrsim 0.5$ s) longer than the mean interbeat ($\sim 10^{-1}$ s). We have also reported the results of a two-point magnitude correlation analysis which infers the absence of a multiplicative time-scale structure underlying multifractal scaling. The electric energy dynamics looks like a “multifractal white noise” with quadratic (log-normal) multifractal spectra. These observations challenge concepts of functional reentrant circuits in mechanistic theories of AF. A transition is observed in the computed multifractal spectra which group according to two distinct areas, consistently with the anatomical substrate binding to the CS, namely the left atrial posterior wall, and the ligament of Marshall which is innervated by the ANS. These negative results challenge also the existing models, which by principle cannot explain such results. As a consequence, we go beyond the existing models and propose a mathematical model of a denervated heart where the kinetics of gap junction conductance alone induces a desynchronization of the myocardial excitable cells, accounting for the multifractal spectra found experimentally in the left atrial posterior wall area (devoid of ANS influence).

GEOSTAT is focusing on the analysis of turbulent datasets in which the multiscale description can be understood in the form of the multiplicative cascade or, in the case of physiological times series, as excitable systems (cardiac electrophysiology: study of intermittency phenomena). The methodological tools used in reaching these objectives place GEOSTAT at the forefront of nonlinear signal processing and analysis of complex systems. We cite: singularity exponents [56], [7] [11], sparse representations with reconstruction formulae [13] [57], [5], super-resolution in Oceanography and Earth Observation [10], [2], comparison with embedding techniques such as the one provided by the classical theorem of Takens [54], [44], the use of Lyapunov exponents [27] [20], how they are related to intermittency, persistence along the scales [6], comparison with other approaches such as sparse representations and compressive sensing [https://hal.inria.fr/tel-01239958], and the ways that lead to effective numerical and high precision determination of nonlinear characteristics in real signals. Derived from ideas in Statistical Physics, complex signals and systems are studied in relation to the statistical concepts of information content and most informative subsets. As a result, GEOSTAT aims to provide radically new approaches to the study of signals acquired from different complex systems (their analysis, their classification, the study of their dynamical properties etc.). A common characteristic of these signals, which is related to universality classes [48] [49] [45], being the existence of a multiscale organization of the systems. For instance, the classical notion of edge or border, which is of multiscale nature, and whose importance is well known in Computer Vision and Image Processing, receives profound and rigorous new definitions, in relation with the more physical notion of transition fronts/singularities and fits adequately to the case of chaotic data. The description is analogous to the modeling of states far from equilibrium. From this formalism we derive methods able to determine geometrically the most informative part in a signal scale by scale, which also defines its global properties and allows for compact representation. It appears that the notion of transition front in a signal is much more complex than previously expected and, most importantly, related to multiscale notions encountered in the study of nonlinearity [52]. For instance, we give new insights to the computation of dynamical properties in complex signals, in particular in signals for which the classical tools for analyzing dynamics give poor results (such as, for example, correlation methods or optical flow for determining motion in turbulent datasets).
3.2. Excitable systems: analysis of physiological time series

The research described in this section is a collaboration effort of GEOSTAT, CNRS LOMA (Laboratoire Ondes et Matière d’Aquitaine) and Laboratory of Physical Foundation of Strength, Institute of Continuous Media Mechanics (Perm, Russia Federation).

3.2.1. Presentation and objectives

Provide state of the art, cutting-edge tools to intra-cardiac multiscale analysis of the electrical activity of fibrillating hearts; offer physiological hypotheses likely to account for the new quantitative observations together with quantitative simulations.

3.2.2. Results

Wavelet-based methods (WTMM, log-cumulants, two point scale correlations), and confidence statistical methodology, have been applied to catheter recordings in the coronary sinus vein right next to the left atria of a small sample of patients with various conditions, and exhibit clear multifractal scaling without cross-scale correlation, which are coined “multifractal white noise,” and that can be grouped according to two anatomical regions. We show that this is incompatible with the common lore for atrial fibrillation based on so-called circuit reentries. In a new description, we propose that circuit reentries may well exist before the onset of fibrillation, favoring onset but not contributing directly to the onset and perpetuation. By contrast, cell-to-cell coupling is considered fundamentally dynamical. The rationale stems from the observation that multifractal scaling necessitates a high number of degrees of freedom (tending to infinity with system size), which can originate in excitable systems in hyperbolic spatial coupling. In other words, common mathematical models for fibrillation which insist on the intrinsic chaotic dynamics of excitable cells coupled by elliptic propagators (like diffusion) are immune to multifractal scaling. Within this framework, we have developed a new hypothesis in physiology, backed by a mathematical model of gap junction conductance kinetics, that is capable of yielding correct spectra, all based on otherwise known physiology.

3.2.3. Interpretation

Atrial Fibrillation (AF) is an arrhythmia originating in the rapid and irregular electrical activity of the atria (the heart’s two upper chambers) that causes their pump function to fail, increasing up to fivefold the risk of embolic stroke. The rate of AF recurrences after an initial ablation procedure treating paroxysmal AF increases with time, necessitating multiple redos, and most patients suffering persistent AF are resistant to treatment. The prevailing electrophysiological concepts describing tachy-arrhythmias are more than a century old. They involve abnormal automaticity and conduction. Initiation and maintenance are thought to arise from a vulnerable substrate prone to the emergence of multiple self-perpetuating reentry circuits, also called “multiple wavelets”. We have analyzed the complexity of voltage signals recovered with bipolar electrodes in the CS during AF. We used two declinations of a wavelet-based multi-scale method, the moment (partition function) method and the magnitude cumulant method, as originally introduced in the field of fully developed turbulence. In the context of cardiac physiology, this methodology was shown to be valuable in assessing congestive heart failure from the monitoring of sinus heart rate variability (Ivanov, et al. Nature 399, 461–465) [42]. We develop a model such that the substrate function is modulated by the kinetics of conduction. A simple reversible mechanism of short term remodeling under rapid pacing is demonstrated, by which ionic overload acts locally (dynamical feedback) on the kinetics of gap junction conductance. The whole process may propagate and pervade the myocardium via electronic currents, becoming desynchronized. Contrary to existing mathematical models based on circuit reentries, a spatio-temporal multifractal intermittent dynamics emerges similar to the one found in the CS, opening a new avenue towards the understanding of AF mechanisms of perpetuation. We have shown that the wavelet-based multifractal analysis of long time series of the local impulse energy recorded in the CS of a patient with chronic AF was able to reveal and quantify the intermittent nature of these signals at low frequency (f < 2 Hz). To our knowledge, this research is the first to report on the observation and quantification of such multifractal dynamics of the endocavitary electrical activity during AF which is found more complex than previously suspected. Two main observations can be made: (i) the local impulse energy displays different multifractal properties in the left atrial wall area than in the ligament
of Marshall area consistently with different anatomical substrate conditions, and (ii) while recorded along the CS vein, the local impulse energy does not exhibit long-range dependence associated with an underlying multiplicative cascade, or in other words the multifractal distribution of the singularities inferred by the two point magnitude analysis does not display any correlation across scales just like a log-normal “multifractal white noise”.

This analysis definitely challenges current knowledge in physical, physiological and clinical fundamentals of AF arrhythmia.

The absence of an underlying cascading process is not such a surprise since underlying the multifractal properties displayed by the local impulse energy at low frequencies \( f \lessapprox 2 \text{ Hz} \), there is no clear 3D “fragmentation” process inducing some cascading of energy from large to small time scales and also no obvious 2D “aggregation, coalescence or growth” process bringing energy from small to large time scales. What are the physical and physiological mechanisms that drive the multifractal nature of local impulse energy and give rise to the observed differences according to area is still an open question. Nonetheless, these results already undermine the commonly accepted concepts revolving around circuit reentries, and a fortiori spiral waves, as being basic mechanisms for the onset and perpetuation of AF. The mechanistic “wavelength” criterion indeed conveys the idea that random spatio-temporal dispersion of refractoriness, or more generally of functional properties, leads to random mixing of circuit reentries. The “wavelength” scale adjusts naturally to the typical scale \( \lambda \) of dispersion when it exists \( c \times RP \lessapprox \lambda \) as would be the case for Gaussian statistics of dispersion. In that case, the statistics of the local impulse energy remains Gaussian throughout scales. On the contrary, to fit our new observations we see that the statistics is not Gaussian and evolves across scales through a log-normal propagation law, which accounts for the intermittency, over the range of a few beat cycles \( \sim 0,6 \text{ s} \) to several tens \( \sim 10 \text{ s} \) and possibly more), therefore spanning the whole atria. Although the ligament of Marshall area is highly innervated, it is quite unlikely that modulations by the ANS, that affects primarily heart rate, play a significant role in the intermittent dynamics, since the documented three peak frequencies at 0,4 Hz, 0,15 Hz and 0,04 Hz do not show up in our analysis. Furthermore, we have found at least two areas with different multifractal regimes. See figure 1.

Therefore, our findings raise new challenging questions calling for ongoing efforts to develop physiological heart tissue models that account for the low frequency intermittent nature of local impulse energy. In this spirit, in an ongoing research, we propose a model of gap junction conduction remodeling in a denervated heart that accounts for the observed intermittent dynamics over large time scales, as resulting from incoherent random back scatterings, leading to the desynchronization of the network of cardiac excitable cells.

These results have been accepted in a Frontiers in Physiology paper to be published in 2018 https://hal.inria.fr/hal-01673364.

3.3. Multiscale description in terms of multiplicative cascade

GEOSTAT is studying complex signals under the point of view of methods developed in statistical physics to study complex systems, with a strong emphasis on multiresolution analysis. Linear methods in signal processing refer to the standard point of view under which operators are expressed by simple convolutions with impulse responses. Linear methods in signal processing are widely used, from least-square deconvolution methods in adaptive optics to source-filter models in speech processing. Because of the absence of localization of the Fourier transform, linear methods are not successful to unlock the multiscale structures and cascading properties of variables which are of primary importance as stated by the physics of the phenomena. This is the reason why new approaches, such as DFA (Detrented Fluctuation Analysis), Time-frequency analysis, variations on curvelets [53] etc. have appeared during the last decades. Recent advances in dimensionality reduction, and notably in Compressive Sensing, go beyond the Nyquist rate in sampling theory using nonlinear reconstruction, but data reduction occur at random places, independently of geometric localization of information content, which can be very useful for acquisition purposes, but of lower impact in signal analysis. One important result obtained in GEOSTAT is the effective use of multiresolution analysis associated to optimal inference along the scales of a complex system. The multiresolution analysis is performed on dimensionless quantities given by the singularity exponents which encode properly the geometrical structures
Figure 1. $\tau(q)$ spectra of local impulse energy time-series recorded along the CS vein at the electrodes Pt2 (red), Pt3 (blue) and Pt5 (green). The curves represent quadratic polynomial fit of the data. (A) The symbols correspond to the reference Patient 1 (chronic AF), and to Patients 2 (chronic AF), 3 (paroxysmal AF) and 4 (persistent AF). (B) The symbols correspond to the reference Patient 1 and to three different time-series for Patient 4 recorded at different periods of time preceding ablation procedure.

associated to multiscale organization. This is applied successfully in the derivation of high resolution ocean dynamics, or the high resolution mapping of gaseous exchanges between the ocean and the atmosphere; the latter is of primary importance for a quantitative evaluation of global warming. Understanding the dynamics of complex systems is recognized as a new discipline, which makes use of theoretical and methodological foundations coming from nonlinear physics, the study of dynamical systems and many aspects of computer science. One of the challenges is related to the question of emergence in complex systems: large-scale effects measurable macroscopically from a system made of huge numbers of interactive agents [38], [26], [58], [47]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [27]. Consequently, knowledge from acquisitions of complex systems (which include complex signals) could be obtained from information about the phase space. A result from F. Takens [54] about strange attractors in transition turbulence has motivated the determination of discrete dynamical systems associated to time series [44], and consequently the theoretical determination of nonlinear characteristics associated to complex acquisitions. Emergence phenomena can also be traced inside complex signals themselves, by trying to localize information content geometrically. Fundamentally, in the nonlinear analysis of complex signals there are broadly two approaches: characterization by attractors (embedding and bifurcation) and time-frequency, multiscale/multiresolution approaches. Time-frequency analysis [37] and multiscale/multiresolution are the subjects of intense research and are profoundly reshaping the analysis of complex signals by nonlinear approaches [25], [41]. In real situations, the phase space associated to the acquisition of a complex phenomenon is unknown. It is however possible to relate, inside the signal’s domain, local predictability to local reconstruction and deduce from that singularity exponents [11] [7]. We are working on:

- the determination of quantities related to universality classes,
- the geometric localization of multiscale properties in complex signals,
- cascading characteristics of physical variables.

The alternative approach taken in GEOSTAT is microscopical, or geometrical: the multiscale structures which have their "fingerprint" in complex signals are being isolated in a single realization of the complex system, i.e. using the data of the signal itself, as opposed to the consideration of grand ensembles or a wide set of
realizations. This is much harder than the ergodic approaches, but it is possible because a reconstruction formula such as the one derived in [55] is local and reconstruction in the signal's domain is related to predictability. This approach is analogous to the consideration of "microcanonical ensembles" in statistical mechanics.

A multiscale organization is a fundamental feature of a complex system, it can be for example related to the cascading properties in turbulent systems. We make use of this kind of description when analyzing turbulent signals: intermittency is observed within the inertial range and is related to the fact that, in the case of FDT, symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

The example of FDT as a standard "template" for developing general methods that apply to a vast class of complex systems and signals is of fundamental interest because, in FDT, the existence of a multiscale hierarchy \( F_h \) which is of multifractal nature and geometrically localized can be derived from physical considerations. This geometric hierarchy of sets is responsible for the shape of the computed singularity spectra, which in turn is related to the statistical organization of information content in a signal. It explains scale invariance, a characteristic feature of complex signals. The analogy from statistical physics comes from the fact that singularity exponents are direct generalizations of critical exponents which explain the macroscopic properties of a system around critical points, and the quantitative characterization of universality classes, which allow the definition of methods and algorithms that apply to general complex signals and systems, and not only turbulent signals: signals which belong to a same universality class share common statistical organization. In GEOSTAT, the approach to singularity exponents is done within a microcanonical setting, which can interestingly be compared with other approaches such that wavelet leaders, WTMM or DFA. During the past decades, classical approaches (here called "canonical" because they use the analogy taken from the consideration of "canonical ensembles" in statistical mechanics) permitted the development of a well-established analogy taken from thermodynamics in the analysis of complex signals: if \( \mathcal{F} \) is the free energy, \( \mathcal{F} \) the temperature measured in energy units, \( U \) the internal energy per volume unit \( S \) the entropy and \( \beta = 1/T \), then the scaling exponents associated to moments of intensive variables \( p \rightarrow \tau_p \) corresponds to \( \beta \mathcal{F}, U(\beta) \) corresponds to the singularity exponents values, and \( S(U) \) to the singularity spectrum.

The singularity exponents belong to a universality class, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data (where the existence of a multiscale hierarchy, of multifractal nature, can be inferred directly from physical considerations). They describe common multiscale statistical organizations in different complex systems [52], and this is why GEOSTAT is working on nonlinear signal processing tools that are applied to very different types of signals.

For example we give some insight about the collaboration with LEGOS Dynbio team ⁰ about high-resolution ocean dynamics from microcanonical formulations in nonlinear complex signal analysis. Indeed, synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics remains a fundamental challenge in oceanography. This determination has the potential of revealing all aspects of the ocean dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show that the determination of a multiresolution analysis associated to the multiplicative cascade of a typical physical variable like the Sea Surface Temperature permits an optimal inference of oceanic motion field across the scales, resulting in a new method for deriving super resolution oceanic motion from lower resolution altimetry data; the resulting oceanic motion field is validated at super resolution with the use of Lagrangian buoy data available from the Global Drifter Program ⁰. In FDT, singularity exponents range in a bounded interval: \( |h_\infty|, |h_{max}| \) with \( h_\infty < 0 \) being the most singular exponent. Points \( \mathbf{r} \) for which \( h(\mathbf{r}) < 0 \) localize the strongest transition fronts in the turbulent fluid, where an intensive physical variable like sea surface temperature behaves like \( 1/|\mathbf{r}|^{h(\mathbf{r})} \). The links between the geometrically localized singularity exponents, the scaling exponents of structure functions, the multiplicative cascade and the multiscale hierarchy \( F_h \) is the following:

\[ h(\mathbf{r}) = \tau_h \mathcal{F}(\mathbf{r}) \]

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3.4. Data-based identification of characteristic scales and automated modeling

Data are often acquired at the highest possible resolution, but that scale is not necessarily the best for modeling and understanding the system from which data was measured. The intrinsic properties of natural processes do not depend on the arbitrary scale at which data is acquired; yet, usual analysis techniques operate
at the acquisition resolution. When several processes interact at different scales, the identification of their characteristic scales from empirical data becomes a necessary condition for properly modeling the system. A classical method for identifying characteristic scales is to look at the work done by the physical processes, the energy they dissipate over time. The assumption is that this work matches the most important action of each process on the studied natural system, which is usually a reasonable assumption. In the framework of time-frequency analysis [36], the power of the signal can be easily computed in each frequency band, itself matching a temporal scale.

However, in open and dissipative systems, energy dissipation is a prerequisite and thus not necessarily the most useful metric to investigate. In fact, most natural, physical and industrial systems we deal with fall in this category, while balanced quasi-static assumptions are practical approximation only for scales well below the characteristic scale of the involved processes. Open and dissipative systems are not locally constrained by the inevitable rise in entropy, thus allowing the maintaining through time of mesoscopic ordered structures. And, according to information theory [40], more order and less entropy means that these structures have a higher information content than the rest of the system, which usually gives them a high functional role.

We propose to identify characteristic scales not only with energy dissipation, as usual in signal processing analysis, but most importantly with information content. Information theory can be extended to look at which scales are most informative (e.g. multi-scale entropy [31], \( \varepsilon \)-entropy [30]). Complexity measures quantify the presence of structures in the signal (e.g. statistical complexity [33], MPR [46] and others [35]). With these notions, it is already possible to discriminate between random fluctuations and hidden order, such as in chaotic systems [32], [46]. The theory of how information and structures can be defined through scales is not complete yet, but the state of art is promising [34]. Current research in the team focuses on how informative scales can be found using collections of random paths, assumed to capture local structures as they reach out [29].

Building on these notions, it should also possible to fully automate the modeling of a natural system. Once characteristic scales are found, causal relationships can be established empirically. They are then clustered together in internal states of a special kind of Markov models called \( \varepsilon \)-machines [33]. These are known to be the optimal predictors of a system, with the drawback that it is currently quite complicated to build them properly, except for small system [50]. Recent extensions with advanced clustering techniques [28], [39], coupled with the physics of the studied system (e.g. fluid dynamics), have proved that \( \varepsilon \)-machines are applicable to large systems, such as global wind patterns in the atmosphere [43]. Current research in the team focuses on the use of reproducing kernels, coupled possibly with sparse operators, in order to design better algorithms for \( \varepsilon \)-machines reconstruction. In order to help with this long-term project, a collaboration with J. Crutchfield lab at UC Davis was initiated in 2017.

### 3.5. Speech analysis

Our research in speech processing focus on the development of novel nonlinear analysis methods for the characterization and classification of pathological and affective speech. For the latter, classical linear methods do not generally capture the nonlinearity, aperiodicity, turbulence and noise that can be present in pathological voices. We thus aim to design and extract new features that allow better characterization/classification of such voices, while being easy to interpret by clinicians. For the former, recent research have shown that the voice source signal information allow significant improvement of speech emotion detection systems. Our goal is to develop novel nonlinear techniques to extract relevant voice source features and to design efficient machine learning algorithms for robust emotion classification.

### 4. Application Domains

#### 4.1. Analysis of galactic molecular clouds (GENESIS project)

GENESIS (GENeration and Evolution of Structures in the ISm) is a German/French collaboration project, supported for three years (start 1.5. 2017) by the Deutsche Forschungsgemeinde (DFG) and the Agence
national de recherche (ANR). The objective of this research project is to better understand the structure and evolution of molecular clouds in the interstellar medium (ISM) and to link cloud structure with star-formation. For that, far-infrared observations of dust (Herschel) and cooling lines (SOFIA) are combined with ground-based submillimetre observations of molecular lines. Dedicated analysis tools will be used and developed to analyse the maps and compared to simulations in order to disentangle the underlying physical processes such as gravity, turbulence, magnetic fields, and radiation.

4.2. Ocean dynamics, upwelling

Ocean dynamics from remote sensing data is studied in collaboration with LEGOS CNRS Laboratory in Toulouse (SYSCO2) team, with CRTS and Rabat University in Morocco. The following thematics are studied:

- Large time series analysis on global synoptic ocean data to provide fine characteristics of Ocean turbulence, analysis of altimetry data and ocean/atmosphere exchanges (supported by ICARODE project and submitted LEFE-EC2CO IMECO project).
- Upwelling, Lyapunov exponents and Lagrangian Coherent Structures (supported by TOUBKAL project).

4.3. Non convex optimization for image processing

Three years contract with I2S company on sparse representations and non-convex optimizations methods for image processings problems such as: deconvolution, stitching, noise reduction, HDR mapping etc. This contract is taking place after award-winning results of former GEOSTAT PhD student H. Badri.

4.4. Physiological times series: speech processing

Differential diagnosis between Parkinson’s disease and Multiple System Atrophy using complex physiological tile series analysis. Supported by ANR Voice4PD-MSA project.

5. Highlights of the Year

5.1. Highlights of the Year

Innovation LAB GEOSTAT-I2S based on 3 year contract with I2S company on non convex optimization methods for image processing.

5.1.1. Awards

A. Tamim, PhD Student in Geostat, wins the gold medal of Hubert Curien PhD prize 2017. A. Tamim’s PhD title: "Segmentation et classification des images satellitaires : application à la détection des zones d’upwelling côtier marocain et mise en place d’un logiciel de suivi spatiotemporel". See https://www.inria.fr/centre/bordeaux/actualites/prix-de-these-pour-ayoub-tamim.

6. New Software and Platforms

6.1. Fluex

**KEYWORDS:** Signal - Signal processing

**SCIENTIFIC DESCRIPTION:** Fluex is a package consisting of the Microcanonical Multiscale Formalism for 1D, 2D 3D and 3D+t general signals.
**FUNCTIONAL DESCRIPTION:** Fluex is a C++ library developed under Gforge. Fluex is a library in nonlinear signal processing. Fluex is able to analyze turbulent and natural complex signals, Fluex is able to determine low level features in these signals that cannot be determined using standard linear techniques.

- Participants: Hussein Yahia and Rémi Paties
- Contact: Hussein Yahia
- URL: http://fluex.gforge.inria.fr/

### 6.2. FluidExponents

**KEYWORDS:** Signal processing - Wavelets - Fractal - Spectral method - Complexity

**FUNCTIONAL DESCRIPTION:** FluidExponents is a signal processing software dedicated to the analysis of complex signals displaying multiscale properties. It analyzes complex natural signals by use of nonlinear methods. It implements the multifractal formalism and allows various kinds of signal decomposition and reconstruction. One key aspect of the software lies in its ability to evaluate key concepts such as the degree of unpredictability around a point in a signal, and provides different kinds of applications. The software can be used for times series or multidimensional signals.

- Participants: Antonio Turiel and Hussein Yahia
- Contact: Hussein Yahia
- URL: https://fluidexponents@scm.gforge.inria.fr/svn/fluidexponents/FluidExponents

### 6.3. classifemo

**KEYWORDS:** Classification - Audio

**FUNCTIONAL DESCRIPTION:** Classifies vocal audio signals. Classifemo extracts characteristics from vocal audio signals. These characteristics are extracted from signals of different type: initially these were emotion databases, but it can also process signals recorded from patients with motor speech disorders. The software can train usual classifiers (SVM, random forests, etc) on these databases as well as classify new signals.

- Participants: Khalid Daoudi and Nicolas Brodu
- Contact: Khalid Daoudi
- URL: https://allgo.inria.fr/app/emotionclassifierprototype

### 6.4. superres

**Super-Resolution of multi-spectral and multi-resolution images**

**KEYWORD:** Multiscale

**SCIENTIFIC DESCRIPTION:** This resolution enhancement method is designed for multispectral and multiresolution images, such as those provided by the Sentinel-2 satellites (but not only). Starting from the highest resolution bands, band-dependent information (reflectance) is separated from information that is common to all bands (geometry of scene elements). This model is then applied to unmix low-resolution bands, preserving their reflectance, while propagating band-independent information to preserve the sub-pixel details.

**FUNCTIONAL DESCRIPTION:** This super-resolution software for multi-spectral images consists of: - A core C++ library, which can be used directly - A Python module interface to this library - A Java JNI interface to the library - An end-user Python script for super-resolving Sentinel-2 images - An end-user plugin for the widely used SNAP software of the ESA.

- Participant: Nicolas Brodu
- Contact: Nicolas Brodu
- URL: http://nicolas.brodu.net/recherche/superres/index.html

### 6.5. EdgeReconstruct

**Edge Reconstruction With UPM Manifold**
7. New Results

7.1. Multifractal desynchronization of the cardiac excitable cell network during atrial fibrillation

Participants: G. Attuel, H. Yahia.

We compute the so-called multifractal spectra using two variants of the wavelet transform modulus maxima method, the moment (partition function) method and the magnitude cumulant method. Application of these methods to long time series recorded in a patient with chronic AF provides quantitative evidence of the multifractal intermittent nature of the electric energy of passing cardiac impulses at low frequencies, i.e. for times (> 0.5s) longer than the mean interbeat. We also report the results of a two-point magnitude correlation analysis which infers the absence of a multiplicative time-scale structure underlying multifractal scaling. The electric energy dynamics looks like a “multifractal white noise” with quadratic (log-normal) multifractal spectra. These observations challenge concepts of functional reentrant circuits in mechanistic theories of AF, still leaving open the role of the autonomic nervous system (ANS). A transition is indeed observed in the computed multifractal spectra which group according to two distinct areas, consistently with the anatomical substrate binding to the CS, namely the left atrial posterior wall, and the ligament of Marshall which is innervated by the ANS. In a companion paper (II. Modeling), we propose a mathematical model of a denervated heart where the kinetics of gap junction conductance alone induces a desynchronization of the myocardial excitable cells, accounting for the multifractal spectra found experimentally in the left atrial posterior wall area.

Publication: G. Attuel et al., Multifractal desynchronization of the cardiac excitable cell network during atrial fibrillation. I. Multifractal analysis of clinical data. Accepted in Frontiers in Physiology, publication beginning 2018.

7.2. Super-resolution

Participant: N. Brodu.


Publication: [15].

7.3. Surface mixing and biological activity in the Northwest African upwelling

The aim of this work is to study the horizontal stirring and mixing in different upwelling areas of the Northwest African margin using attracting/repelling Lagrangian coherent structures (LCS) obtained as subsets of hyperstreamline of the Cauchy-Green strain tensor, whose normal repulsion rate is larger than tangential stretch over backward/forward time interval, and their link to the chlorophyll fronts concentrations, based on 10 years satellite data. The temporal variability of surface stirring is compared to the fronts chlorophyll concentration. Two of the four studied areas exhibit negative correlation between mixing and the chlorophyll concentration. The other two regions show similar seasonal variations, nearly coincident maxima and minima, leading to a global positive correlation. These results are compared to other works that make use of Finite Size Lyapunov Exponent (FSLE) whose output is a plot of scalar distributions. Furthermore, we compare the chlorophyll concentrations with both compressing and stretching lines. Results show different regions with different properties. The surface mixing and chlorophyll concentrations correlation is governed by stretching lines in two regions, by compressing lines in one region with, while no different is shown between attracting and repelling LCS in the northern region of the studied area.

Publication: [20].

7.4. Spatio-Temporal Dynamics of Floods

Participant: N. Brodu.

The floods are an annual phenomenon on the Pacific Coast of Ecuador and can become devastating during El Niño years, especially in the Guayas watershed (32,300 km²), the largest drainage basin of the South American western side of the Andes. As limited information on flood extent in this basin is available, this study presents a monitoring of the spatio-temporal dynamics of floods in the Guayas Basin, between 2005 and 2008, using a change detection method applied to ENVISAT ASAR Global Monitoring SAR images acquired at a spatial resolution of 1 km.

Publication: [16].

7.5. Effect of wind stress forcing on ocean dynamics at Air-Sea Interface

Participant: H. Yahia.

At first order, oceanic currents are generated by the balance of Coriolis and pressure gradient (geostrophic current) and the balance of Coriolis and the frictional force dominated by wind stress in the surface ocean (Ekman current). We aim at studying the difference in term of turbulent hydrodynamics carried by the wind forcing at the air-sea interface. We explore the statistical properties of singularity spectra computed from velocity norms and vorticity data, notably in relation with kurtosis information to underline differences in the turbulent regimes associated with both kinds of velocity fields. This study is conducted over 1 year of daily data and demonstrates the differences in terms of turbulent property of wind forcing.

Publication: [24].

7.6. Ocean dynamics: frontal activity

Participant: H. Yahia.

A highresolution (1km spatial and daily temporal resolutions) dataset of 11 years (2003 to 2013) remotely sensed SST by MODIS sensor onboard Aqua and Terra satellites has been investigated and compared with coastal numerical model experiments. The detection and characterization fronts with fluctuating amplitudes is achieved through the Singularity Analysis (i.e. the process of calculating the degree of regularity or irregularity of a function at each point in a domain).

Publication: [18].
7.7. Pathological speech processing

Participants: K. Daoudi, G. Li, Q. Robin, F. G. Satsou.

- Small amount of training data in learning robust classifiers for differential diagnosis between progressive supranuclear palsy (PSP) and multiple system atrophy (MSA). We showed that factorial discriminant analysis and logistic regression can lead to such robust classifiers. Moreover, we showed that these models provide good insights on the multivariate variability and (un)correlation of acoustic features, which can facilitate clinical interpretation.

- We investigated the problem of extracting ground truth of glottal closure instants (GCI) from electroglottographic (EGG) signals of healthy and pathological speakers. We carried out a large experimental study which showed that existing methods are not robust to recording settings and material. We then proposed a method to overcome this problem. On the other hand, this problem highlighted the non robustness of state of the art methods in automatic detection of GCI from speech.

- We made an experimental evaluation of state of the art methods in automatic extraction of the excitation source from voiced speech. To carry out this evaluation, we used a very recent source-filter model of sustained phonations. The results showed that these methods are reliable only in very particular cases and fail in most.

- Matching pursuit (MP), particularly using the Gammatones dictionary, has become a popular tool in sparse representations of speech/audio signals. The classical MP algorithm does not however take into account psychoacoustical aspects of the auditory system. Recently two algorithms, called PAMP and PMP have been introduced in order to select only perceptually relevant atoms during MP decomposition. We compared the performance these two algorithms on few speech sentences. The results showed that PMP, which also has the strong advantage of including an implicit stop criterion, always outperforms PAMP as well as classical MP. We then raised the question of whether the Gammatones dictionary is the best choice when using PMP. We thus compared it to the popular Gabor and damped-Sinusoids dictionaries. The results showed that Gammatones always outperform damped-Sinusoids, and that Gabor yield better reconstruction quality but with higher atoms rate.

Publications: [22], [23], [21], [19].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Three year contract with I2S company on the transfert of award winning H. Badri PhD results (AFRIF PhD price in 2016). The contract is being transformed in 2018 in the form of an Inria Innovation Lab. The Innovation Lab is focused on non convex optimization methods in image processing and digital acquisition devices. People involved in GEOSTAT: H. Yahia, N. Brodu, K. Daoudi, M. Martin, A. Zebadua.

8.2. Bilateral Grants with Industry

- Transfert in the analysis of hearbeat data. Discussion and collaboration with Cardiologs company https://cardiologs.com/.
- Contacts for a partnership strategy on heartbeat database utilization with Purly II Hospital (F. Halimi).
- Patent 185 "Dispositif analyseur de rythme cardiaque” extended for France in 2018.
9. Partnerships and Cooperations

9.1. Regional Initiatives

GEOSTAT is working with the following regional partners:

- CNRS LOMA (Laboratoire Ondes et Matière d’Aquitaine) and RAS Institute (Russia): collaboration on the analysis/modeling of heartbeat physiological time series (A. Arneodo, E. Gerasimova, F. Argoul).
- GEOSTAT has a decade-long close scientific collaboration with team SYSCO2 (LEGOS Laboratoire UMR 5566): V. Garçon, B. Dewitte, J. Sudre.
- Laboratoire d’Astrophysique de Bordeaux (S. Bontemps, N. Schneider, GENESIS project).
- Collaboration with L. Bourrel (GET Toulouse / IRD) and F. Frappart (GET/UMR EPOC) Flood monitoring in Equator.
- With Bruno Castelle (EPOC).
- With D. Gibert (OSUR) on signal and image processing.
- CHU Bordeaux: Prof. Wassilios Meissner (IMN), Dr. Solange Milhée de Saint Victor (service ORL).
- CHU Toulouse: Dr. Anne Pavy Le traon (service Neurologie), Prof. Virginie Woisard (service ORL).
- IRIT: Prof. Régine André-Obrecht, Dr. Julie Mauclair.
- IMT (Institut de Mathématique de Toulouse): Dr. Sébastien Déjean, Dr. Laurent Risser.
- Mercator Océan: Dr. A. El Moussaoui. UMR EPOC).

9.2. National Initiatives

- ANR project Voice4PD-MSA, led by K. Daoudi, which targets the differential diagnosis between Parkinson’s disease and Multiple System Atrophy. The total amount of the grant is 468555 euros, from which GeoStat has 203078 euros. The duration of the project is 42 months. Partners: CHU Bordeaux (Bordeaux), CHU Toulouse, IRIT, IMT (Toulouse).
- PhD grant for C. Artnana from UPMC University, under co-supervision with H. Yahia and C. Provost (LOCEAN, Paris).
- PhD grant for G. Singh from IIT Roorkee, under co-supervision with D. Singh (IIT Roorkee).
- The PHC-Toubkal project “Caractérisation multi-capteurs et suivi spatio-temporel de l’Upwelling sur la côte atlantique marocaine par imagerie satellitaire”, led by K. Daoudi, is in its second year. The partners in this project are: Faculté des sciences de Rabat, Centre Royal de Télédétection Spatiale, Mercator-Ocean and GEOSTAT.
- GEOSTAT is a member of ISIS (Information, Image & Vision) and AMF (Multifractal Analysis) GDRs.

9.3. European Initiatives

9.3.1. Collaborations in European Programs, Except FP7 & H2020

Program: supported by Deutsche Forschungsgemeinde (DFG) and the Agence national de recherche (ANR).

Project acronym: GENESIS.

Project title: GENeration and Evolution of Structures in the ISm.

Duration: start 1.5. 2017, 3 years.

Coordinator: N. Schneider (I. Physik, Cologne).
Abstract: The formation of stars is intimately linked to the structure and evolution of molecular clouds in the interstellar medium (ISM). We propose to explore this link with a new approach by combining far infrared maps of dust (Herschel) and cooling lines (C+ with SOFIA) with molecular line maps. Dedicated analysis tools will be used and developed to analyze the maps and compare them to simulations in order to identify for the underlying physical processes. This joint project relies on the complementary expertise of the members of the Cologne KOSMA group (structure identification methods and SOFIA), the Bordeaux LAB star formation group (Herschel and spectro-imaging maps), and the Bordeaux GEOSTAT team of Inria. To understand the genesis of stars, it is necessary to disentangle the relative importance of gravity, turbulence, magnetic fields, and radiation from diffuse gas, to molecular clouds and collapsing cores, and to study the role of filaments. Using innovative new analyzing tools developed by the GeoStat team, we will analyze the Herschel images as well as new spectro-imaging surveys from ground-based telescopes, and THz spectroscopy using SOFIA. The comparison with similar analysis on simulated clouds will allow us to derive the underlying physical process which explains cloud evolution and the formation of dense structures. The project does not aim at a full understanding of star formation within 3 years, but it constitutes an important step forward as it will make systematic use of a wealth of existing, yet not fully exploited archival data, carefully chosen new observations, and sophisticated tools to analyze and interpret the data. As such, it will shed new light on how molecular clouds and stars form and may well be the starting point for many studies to follow.

9.4. International Initiatives

9.4.1. Inria International Partners

Funding from French-Indian IFCAM program (Visit of Prof. D. Singh in GEOSTAT, 2017).

9.4.1.1. Informal International Partners

- Visit of N. Brodu to Univ. UC Davis in the team of Prof. J. Crutchfield. Setting up of a collaboration on a formalism of statistical reconstruction from dynamic empirical data; the formalism involves markovian automata called Epsilon machines. The internal states of these machine correspond to equivalence classes of a physical system having similar causal relations.
- Laboratory LRIT from Rabat University (K. Minaoui, D. Aboutajdine).

9.4.2. Participation in Other International Programs

Participation in the IFCAM project with India (funding of the visit of Prof. D. Singh in 2017).

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- N. Schneider (Cologne University, GENESIS project).
- Prof. D. Singh (IIT roorkee, on CEFIPRA-CNRS funding). Duration: 8 weeks, August and December 2017. Co-supervision of G. Singh PhD student, scientific collaboration with N. Brodu and K. Daoudi.

9.5.1.1. Internships

- G. Li. Master2, University Paris-Saclay.
- Q. Robin. Engineer, INP-Grenble.
9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

June-July 2017: PhD student A. El Aouni was invited in the MERCATOR project by A. Moussaoui in the framework of the Toubkal project on ocean modeling.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees


10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

H. Yahia is a review editor of Frontiers in Fractal Physiology.

10.1.2.2. Reviewer - Reviewing Activities

H. Yahia: Frontiers in Physiology.

10.1.3. Invited Talks

- K. Daoudi has been invited to the Wolrd Voice Consortium 2017 to present the project on differential diagnosis in Parkinsonism.
- H. Yahia: presentation given to the Laboratoire d’Astrophysioique de Bordeaux on March 8, 2017.
- A. Tamim is invited in June 2017 for the reception of his PHC Hubert Curien PhD gold medal.
- Visit of D. Singh in GEOSTAT in August 2017 on the co-supervision of G. Singh PhD thesis.
- Invitation of H. Badri in the framework of I2S kickoff meeting, on Inria funding.

10.1.4. Research Administration

- Participation of H. Yahia, H. Badri, K. Daoudi and N. Brodu to the I2S-GEOSTAT kickoff meeting in September 2017.
- Participation of K. Daoudi to the SABOR project organization.

10.2. Teaching - Supervision - Juries

10.2.1. Supervision

- F. G. Satsou. Master1, University Bordeaux 1.
PhD in progress: B. Das, supervised of H. Yahia in the framework of the Toubkal project (starts 01/01/18).
PhD in progress: A. El Aouni, co-supervised by K. Daoudi, H. Yahia and K. Minaoui in the framework of the Toubkal project.
PhD in progress: G. Singh, co-supervised by N. Brodù in the framework of OPTIC associated team anf IFCAM collaboration.
PhD in progress: C. Artana, co-supervised by H. Yahia in a collaboration with LOCEAN team (Univ. Paris 6).

10.3. Popularization

Diffusion of the GENESIS project in the magazine Inria PLUGIN (published begining 2018) and in the Inria website (national and INRIS BSO), see https://www.inria.fr/centre/bordeaux/actualites/lancement-du-projet-genesis.

11. Bibliography

Major publications by the team in recent years


Publications of the year
Articles in International Peer-Reviewed Journal


International Conferences with Proceedings


Other Publications


[22] G. Li. *Speech analysis for the differential diagnosis between Parkinson’s disease, progressive supranuclear palsy and multiple system atrophy*, Université Paris Saclay, September 2017, https://hal.inria.fr/hal-01627868.


References in notes


Project-Team HIEPACS

High-End Parallel Algorithms for Challenging Numerical Simulations

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS
Institut Polytechnique de Bordeaux
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing
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Project-Team HIEPACS

Creation of the Team: 2009 January 01, updated into Project-Team: 2010 January 01

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Computer Science and Digital Science:
  A1.1.4. - High performance computing
  A1.1.5. - Exascale
  A6.2.5. - Numerical Linear Algebra
  A6.2.7. - High performance computing
  A7.1. - Algorithms
  A8.1. - Discrete mathematics, combinatorics

Other Research Topics and Application Domains:
  B3.3.1. - Earth and subsoil
  B3.4.2. - Industrial risks and waste
  B4.1. - Fossil energy production (oil, gas)
  B4.2.2. - Fusion
  B5.5. - Materials
  B9.4.1. - Computer science
  B9.4.2. - Mathematics
  B9.4.4. - Chemistry

1. Personnel

Research Scientists
  Luc Giraud [Team leader, Inria, Senior Researcher, HDR]
  Emmanuel Agullo [Inria, Researcher]
  Olivier Coulaud [Inria, Senior Researcher, HDR]
  Jean Roman [Inria, Senior Researcher, HDR]

Faculty Members
  Aurélien Esnard [Univ de Bordeaux, Associate Professor]
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  Pierre Ramet [Univ Bordeaux I, Associate Professor, HDR]

External Collaborators
  Maria Predari [Univ de Bordeaux, until Jun 2017]
  Guillaume Sylvand [Airbus Group]

Technical Staff
  Yuval Harness [Inria, until Jun 2017]
  Matias Hastaran [Inria, granted by PRACE 4IP until Feb 2017]
  Quentin Khan [Inria, until Apr 2017]
  Matthieu Kuhn [Inria, granted by H2020 HPC4E]
  Gilles Marait [Inria, granted by H2020 EoCoE]
  Cyrille Piacibello [Inria, granted by DGA HiBox until Apr 2017]

PhD Students
2. Overall Objectives

2.1. Introduction

Over the last few decades, there have been innumerable science, engineering and societal breakthroughs enabled by the development of high performance computing (HPC) applications, algorithms and architectures. These powerful tools have provided researchers with the ability to computationally find efficient solutions for some of the most challenging scientific questions and problems in medicine and biology, climatology, nanotechnology, energy and environment. It is admitted today that numerical simulation is the third pillar for the development of scientific discovery at the same level as theory and experimentation. Numerous reports and papers also confirmed that very high performance simulation will open new opportunities not only for research but also for a large spectrum of industrial sectors.

An important force which has continued to drive HPC has been to focus on frontier milestones which consist in technical goals that symbolize the next stage of progress in the field. In the 1990s, the HPC community sought to achieve computing at a teraflop rate and currently we are able to compute on the first leading architectures at a petaflop rate. Generalist petaflop supercomputers are available and exaflop computers are foreseen in early 2020.

For application codes to sustain petaflops and more in the next few years, hundreds of thousands of processor cores or more are needed, regardless of processor technology. Currently, a few HPC simulation codes easily scale to this regime and major algorithms and codes development efforts are critical to achieve the potential of these new systems. Scaling to a petaflop and more involves improving physical models, mathematical modeling, super scalable algorithms that will require paying particular attention to acquisition, management and visualization of huge amounts of scientific data.

In this context, the purpose of the HiEPACS project is to contribute performing efficiently frontier simulations arising from challenging academic and industrial research. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on emerging hierarchical many-core, possibly heterogeneous, platforms. Through this approach, HiEPACS intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers. This research will be conducted on close collaboration in particular with European and US initiatives and likely in the framework of H2020 European collaborative projects.
The methodological part of HiEPAI covers several topics. First, we address generic studies concerning massively parallel computing, the design of high-end performance algorithms and software to be executed on future extreme scale platforms. Next, several research prospectives in scalable parallel linear algebra techniques are addressed, ranging from dense direct, sparse direct, iterative and hybrid approaches for large linear systems. Then we consider research on N-body interaction computations based on efficient parallel fast multipole methods and finally, we address research tracks related to the algorithmic challenges for complex code couplings in multiscale/multiphysic simulations.

Currently, we have one major multiscale application that is in material physics. We contribute to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modeling and our advanced numerical schemes will help in the design and efficient software implementation for very large parallel multiscale simulations. Moreover, the robustness and efficiency of our algorithmic research in linear algebra are validated through industrial and academic collaborations with different partners involved in various application fields. Finally, we are also involved in a few collaborative initiatives in various application domains in a co-design like framework. These research activities are conducted in a wider multi-disciplinary context with colleagues in other academic or industrial groups where our contribution is related to our expertise. Not only these collaborations enable our knowledge to have a stronger impact in various application domains through the promotion of advanced algorithms, methodologies or tools, but in return they open new avenues for research in the continuity of our core research activities.

Thanks to the two Inria collaborative agreements such as with Airbus Group/Conseil Régional Grande Aquitaine and with CEA, we have joint research efforts in a co-design framework enabling efficient and effective technological transfer towards industrial R&D. Furthermore, thanks to the ending associate team FASTLA we contribute with world leading groups at Berkeley National Lab and Stanford University to the design of fast numerical solvers and their parallel implementations.

Our high performance software packages are integrated in several academic or industrial complex codes and are validated on very large scale simulations. For all our software developments, we use first the experimental platform PLAIFRIM, the various large parallel platforms available through GENCI in France (CCRT, CINES and IDRIS Computational Centers), and next the high-end parallel platforms that will be available via European and US initiatives or projects such that PRACE.

3. Research Program

3.1. Introduction

The methodological component of HiEPAI concerns the expertise for the design as well as the efficient and scalable implementation of highly parallel numerical algorithms to perform frontier simulations. In order to address these computational challenges, a hierarchical organization of the research is considered. In this bottom-up approach, we first consider in Section 3.2 generic topics concerning high performance computational science. The activities described in this section are transversal to the overall project and their outcome will support all the other research activities at various levels in order to ensure the parallel scalability of the algorithms. The aim of this activity is not to study general purpose solution but rather to address these problems in close relation with specialists of the field in order to adapt and tune advanced approaches in our algorithmic designs. The next activity, described in Section 3.3, is related to the study of parallel linear algebra techniques that currently appear as promising approaches to tackle huge problems on extreme scale platforms. We highlight the linear problems (linear systems or eigenproblems) because they are in many large scale applications the main computational intensive numerical kernels and often the main performance bottleneck. These parallel numerical techniques will be the basis of both academic and industrial collaborations, some are described in Section 4.1, but will also be closely related to some functionalities developed in the parallel fast multipole activity described in Section 3.4. Finally, as the accuracy of the physical models increases, there is a real need to go for parallel efficient algorithm implementation for multiphysics and multiscale modeling in particular in the context of code coupling. The challenges associated with this activity will be addressed in the framework of the activity described in Section 3.5.
Currently, we have one major application (see Section 4.1) that is in material physics. We will collaborate to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modelling, our advanced numerical schemes will help in the design and efficient software implementation for very large parallel simulations. We also participate to a few co-design actions in close collaboration with some applicative groups. The objective of this activity is to instantiate our expertise in fields where they are critical for designing scalable simulation tools. We refer to Section 4.2 for a detailed description of these activities.

3.2. High-performance computing on next generation architectures

**Participants:** Emmanuel Agullo, Olivier Coulaud, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Matias Hastaran, Grégoire Pichon, Pierre Ramet, Jean Roman.

The research directions proposed in HiEPACS are strongly influenced by both the applications we are studying and the architectures that we target (i.e., massively parallel heterogeneous many-core architectures, ...). Our main goal is to study the methodology needed to efficiently exploit the new generation of high-performance computers with all the constraints that it induces. To achieve this high-performance with complex applications we have to study both algorithmic problems and the impact of the architectures on the algorithm design.

From the application point of view, the project will be interested in multiresolution, multiscale and hierarchical approaches which lead to multi-level parallelism schemes. This hierarchical parallelism approach is necessary to achieve good performance and high-scalability on modern massively parallel platforms. In this context, more specific algorithmic problems are very important to obtain high performance. Indeed, the kind of applications we are interested in are often based on data redistribution for example (e.g., code coupling applications). This well-known issue becomes very challenging with the increase of both the number of computational nodes and the amount of data. Thus, we have both to study new algorithms and to adapt the existing ones. In addition, some issues like task scheduling have to be restudied in this new context. It is important to note that the work developed in this area will be applied for example in the context of code coupling (see Section 3.5).

Considering the log.html of modern architectures like massively parallel architectures or new generation heterogeneous multicore architectures, task scheduling becomes a challenging problem which is central to obtain a high efficiency. Of course, this work requires the use/design of scheduling algorithms and models specifically to tackle our target problems. This has to be done in collaboration with our colleagues from the scheduling community like for example O. Beaumont (Inria REALOPT Project-Team). It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore architectures, it has appeared, in the last five years, that the best programming model is an approach mixing multi-threading within computational nodes and message passing between them. In the last five years, a lot of work has been developed in the high-performance computing community to understand what is critic to efficiently exploit massively multicore platforms that will appear in the near future. It appeared that the key for the performance is firstly the granularity of the computations. Indeed, in such platforms the granularity of the parallelism must be small so that we can feed all the computing units with a sufficient amount of work. It is thus very crucial for us to design new high performance tools for scientific computing in this new context. This will be developed in the context of our solvers, for example, to adapt to this new parallel scheme. Secondly, the larger the number of cores inside a node, the more complex the memory hierarchy. This remark impacts the behaviour of the algorithms within the node. Indeed, on this kind of platforms, NUMA effects will be more and more problematic. Thus, it is very important to study and design data-aware algorithms which take into account the affinity between computational threads and the data they access. This is particularly important in the context of our high-performance tools. Note that this work has to be based on an intelligent cooperative underlying run-time (like the tools developed by the Inria STORM Project-Team) which allows a fine management of data distribution within a node.

Another very important issue concerns high-performance computing using “heterogeneous” resources within a computational node. Indeed, with the deployment of the GPU and the use of more specific co-processors, it is important for our algorithms to efficiently exploit these new type of architectures. To adapt our algorithms
and tools to these accelerators, we need to identify what can be done on the GPU for example and what cannot. Note that recent results in the field have shown the interest of using both regular cores and GPU to perform computations. Note also that in opposition to the case of the parallelism granularity needed by regular multicore architectures, GPU requires coarser grain parallelism. Thus, making both GPU and regular cores work all together will lead to two types of tasks in terms of granularity. This represents a challenging problem especially in terms of scheduling. From this perspective, we investigate new approaches for composing parallel applications within a runtime system for heterogeneous platforms.

In that framework, the SOLHAR project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computers equipped with accelerators. Several attempts have been made to accomplish the porting of these methods on such architectures; the proposed approaches are mostly based on a simple offloading of some computational tasks (the coarsest grained ones) to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. SOLHAR proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool developed in the STORM team. Although the SOLHAR project will focus on heterogeneous computers equipped with GPUs due to their wide availability and affordable cost, the research accomplished on algorithms, methods and programming models will be readily applicable to other accelerator devices. Our final goal would be to have high performance solvers and tools which can efficiently run on all these types of complex architectures by exploiting all the resources of the platform (even if they are heterogeneous).

In order to achieve an advanced knowledge concerning the design of efficient computational kernels to be used on our high performance algorithms and codes, we will develop research activities first on regular frameworks before extending them to more irregular and complex situations. In particular, we will work first on optimized dense linear algebra kernels and we will use them in our more complicated direct and hybrid solvers for sparse linear algebra and in our fast multipole algorithms for interaction computations. In this context, we will participate to the development of those kernels in collaboration with groups specialized in dense linear algebra. In particular, we intend develop a strong collaboration with the group of Jack Dongarra at the University of Tennessee and collaborating research groups. The objectives will be to develop dense linear algebra algorithms and libraries for multicore architectures in the context the PLASMA project and for GPU and hybrid multicore/GPU architectures in the context of the MAGMA project. A new solver has emerged from the associate team, Chameleon. While PLASMA and MAGMA focus on multicore and GPU architectures, respectively, Chameleon makes the most out of heterogeneous architectures thanks to task-based dynamic runtime systems.

A more prospective objective is to study the resiliency in the context of large-scale scientific applications for massively parallel architectures. Indeed, with the increase of the number of computational cores per node, the probability of a hardware crash on a core or of a memory corruption is dramatically increased. This represents a crucial problem that needs to be addressed. However, we will only study it at the algorithmic/application level even if it needed lower-level mechanisms (at OS level or even hardware level). Of course, this work can be performed at lower levels (at operating system) level for example but we do believe that handling faults at the application level provides more knowledge about what has to be done (at application level we know what is critical and what is not). The approach that we will follow will be based on the use of a combination of fault-tolerant implementations of the run-time environments we use (like for example ULFM) and an adaptation of our algorithms to try to manage this kind of faults. This topic represents a very long range objective which needs to be addressed to guaranty the robustness of our solvers and applications.

Finally, it is important to note that the main goal of HiePACS is to design tools and algorithms that will be used within complex simulation frameworks on next-generation parallel machines. Thus, we intend with our partners to use the proposed approach in complex scientific codes and to validate them within very large scale simulations as well as designing parallel solution in co-design collaborations.

### 3.3. High performance solvers for large linear algebra problems
Participants: Emmanuel Agullo, Olivier Coulaud, Mathieu Faverge, Aurélien Falco, Luc Giraud, Abdou Guermouche, Yuval Harness, Matias Hastaran, Matthieu Kuhn, Gilles Marait, Cyrille Piacibello, Grégoire Pichon, Louis Poirel, Pierre Ramet, Jean Roman, Cristobal Samaniego Alvarado, Guillaume Sylvand.

Starting with the developments of basic linear algebra kernels tuned for various classes of computers, a significant knowledge on the basic concepts for implementations on high-performance scientific computers has been accumulated. Further knowledge has been acquired through the design of more sophisticated linear algebra algorithms fully exploiting those basic intensive computational kernels. In that context, we still look at the development of new computing platforms and their associated programming tools. This enables us to identify the possible bottlenecks of new computer architectures (memory path, various level of caches, inter processor or node network) and to propose ways to overcome them in algorithmic design. With the goal of designing efficient scalable linear algebra solvers for large scale applications, various tracks will be followed in order to investigate different complementary approaches. Sparse direct solvers have been for years the methods of choice for solving linear systems of equations, it is nowadays admitted that classical approaches are not scalable neither from a computational complexity nor from a memory view point for large problems such as those arising from the discretization of large 3D PDE problems. We will continue to work on sparse direct solvers on the one hand to make sure they fully benefit from most advanced computing platforms and on the other hand to attempt to reduce their memory and computational costs for some classes of problems where data sparse ideas can be considered. Furthermore, sparse direct solvers are a key building boxes for the design of some of our parallel algorithms such as the hybrid solvers described in the sequel of this section. Our activities in that context will mainly address preconditioned Krylov subspace methods; both components, preconditioner and Krylov solvers, will be investigated. In this framework, and possibly in relation with the research activity on fast multipole, we intend to study how emerging H-matrix arithmetic can benefit to our solver research efforts.

3.3.1. Parallel sparse direct solver

For the solution of large sparse linear systems, we design numerical schemes and software packages for direct and hybrid parallel solvers. Sparse direct solvers are mandatory when the linear system is very ill-conditioned; such a situation is often encountered in structural mechanics codes, for example. Therefore, to obtain an industrial software tool that must be robust and versatile, high-performance sparse direct solvers are mandatory, and parallelism is then necessary for reasons of memory capability and acceptable solution time. Moreover, in order to solve efficiently 3D problems with more than 50 million unknowns, which is now a reachable challenge with new multicore supercomputers, we must achieve good scalability in time and control memory overhead. Solving a sparse linear system by a direct method is generally a highly irregular problem that induces some challenging algorithmic problems and requires a sophisticated implementation scheme in order to fully exploit the capabilities of modern supercomputers.

New supercomputers incorporate many microprocessors which are composed of one or many computational cores. These new architectures induce strongly hierarchical topologies. These are called NUMA architectures. In the context of distributed NUMA architectures, in collaboration with the Inria STORM team, we study optimization strategies to improve the scheduling of communications, threads and I/O. We have developed dynamic scheduling designed for NUMA architectures in the PaStiX solver. The data structures of the solver, as well as the patterns of communication have been modified to meet the needs of these architectures and dynamic scheduling. We are also interested in the dynamic adaptation of the computation grain to use efficiently multi-core architectures and shared memory. Experiments on several numerical test cases have been performed to prove the efficiency of the approach on different architectures. Sparse direct solvers such as PaStiX are currently limited by their memory requirements and computational cost. They are competitive for small matrices but are often less efficient than iterative methods for large matrices in terms of memory. We are currently accelerating the dense algebra components of direct solvers using hierarchical matrices algebra.

In collaboration with the ICL team from the University of Tennessee, and the STORM team from Inria, we are evaluating the way to replace the embedded scheduling driver of the PaStiX solver by one of the generic frameworks, PaRSEC or StarPU, to execute the task graph corresponding to a sparse factorization. The aim...
is to design algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with GPU accelerators. More generally, this work will be performed in the context of the ANR SOLHAR project which aims at designing high performance sparse direct solvers for modern heterogeneous systems. This ANR project involves several groups working either on the sparse linear solver aspects (HIEPACS and ROMA from Inria and APO from IRIT), on runtime systems (STORM from Inria) or scheduling algorithms (REALOPT and ROMA from Inria). The results of these efforts will be validated in the applications provided by the industrial project members, namely CEA-CESTA and Airbus Group Innovations.

3.3.2. Hybrid direct/iterative solvers based on algebraic domain decomposition techniques

One route to the parallel scalable solution of large sparse linear systems in parallel scientific computing is the use of hybrid methods that hierarchically combine direct and iterative methods. These techniques inherit the advantages of each approach, namely the limited amount of memory and natural parallelization for the iterative component and the numerical robustness of the direct part. The general underlying ideas are not new since they have been intensively used to design domain decomposition techniques; those approaches cover a fairly large range of computing techniques for the numerical solution of partial differential equations (PDEs) in time and space. Generally speaking, it refers to the splitting of the computational domain into sub-domains with or without overlap. The splitting strategy is generally governed by various constraints/objectives but the main one is to express parallelism. The numerical properties of the PDEs to be solved are usually intensively exploited at the continuous or discrete levels to design the numerical algorithms so that the resulting specialized technique will only work for the class of linear systems associated with the targeted PDE.

In that context, we continue our effort on the design of algebraic non-overlapping domain decomposition techniques that rely on the solution of a Schur complement system defined on the interface introduced by the partitioning of the adjacency graph of the sparse matrix associated with the linear system. Although it is better conditioned than the original system the Schur complement needs to be precondition to be amenable to a solution using a Krylov subspace method. Different hierarchical preconditioners will be considered, possibly multilevel, to improve the numerical behaviour of the current approaches implemented in our software libraries HIPS and MaPHyS. This activity will be developed in the context of the ANR DEDALES project. In addition to this numerical studies, advanced parallel implementation will be developed that will involve close collaborations between the hybrid and sparse direct activities.

3.3.3. Linear Krylov solvers

Preconditioning is the main focus of the two activities described above. They aim at speeding up the convergence of a Krylov subspace method that is the complementary component involved in the solvers of interest for us. In that framework, we believe that various aspects deserve to be investigated; we will consider the following ones:

- preconditioned block Krylov solvers for multiple right-hand sides. In many large scientific and industrial applications, one has to solve a sequence of linear systems with several right-hand sides given simultaneously or in sequence (radar cross section calculation in electromagnetism, various source locations in seismic, parametric studies in general, ...). For “simultaneous” right-hand sides, the solvers of choice have been for years based on matrix factorizations as the factorization is performed once and simple and cheap block forward/backward substitutions are then performed. In order to effectively propose alternative to such solvers, we need to have efficient preconditioned Krylov subspace solvers. In that framework, block Krylov approaches, where the Krylov spaces associated with each right-hand side are shared to enlarge the search space will be considered. They are not only attractive because of this numerical feature (larger search space), but also from an implementation point of view. Their block-structures exhibit nice features with respect to data locality and re-usability that comply with the memory constraint of multicore architectures. We will continue the numerical study and design of the block GMRES variant that combines inexact breakdown detection, deflation at restart and subspace recycling. Beyond new numerical investigations, a software implementation to be included in our linear solver library Fabulous originally developed
in the context of the DGA HiBox project.

• Extension or modification of Krylov subspace algorithms for multicore architectures: finally to match as much as possible to the computer architecture evolution and get as much as possible performance out of the computer, a particular attention will be paid to adapt, extend or develop numerical schemes that comply with the efficiency constraints associated with the available computers. Nowadays, multicore architectures seem to become widely used, where memory latency and bandwidth are the main bottlenecks; investigations on communication avoiding techniques will be undertaken in the framework of preconditioned Krylov subspace solvers as a general guideline for all the items mentioned above.

3.3.4. Eigensolvers

Many eigensolvers also rely on Krylov subspace techniques. Naturally some links exist between the Krylov subspace linear solvers and the Krylov subspace eigensolvers. We plan to study the computation of eigenvalue problems with respect to the following two different axes:

• Exploiting the link between Krylov subspace methods for linear system solution and eigensolvers, we intend to develop advanced iterative linear methods based on Krylov subspace methods that use some spectral information to build part of a subspace to be recycled, either through space augmentation or through preconditioner update. This spectral information may correspond to a certain part of the spectrum of the original large matrix or to some approximations of the eigenvalues obtained by solving a reduced eigenproblem. This technique will also be investigated in the framework of block Krylov subspace methods.

• In the context of the calculation of the ground state of an atomistic system, eigenvalue computation is a critical step; more accurate and more efficient parallel and scalable eigensolvers are required.

3.4. High performance Fast Multipole Method for N-body problems

Participants: Emmanuel Agullo, Pierre Blanchard, Olivier Coulaud, Quentin Khan, Guillaume Sylvand.

In most scientific computing applications considered nowadays as computational challenges (like biological and material systems, astrophysics or electromagnetism), the introduction of hierarchical methods based on an octree structure has dramatically reduced the amount of computation needed to simulate those systems for a given accuracy. For instance, in the N-body problem arising from these application fields, we must compute all pairwise interactions among N objects (particles, lines, ...) at every timestep. Among these methods, the Fast Multipole Method (FMM) developed for gravitational potentials in astrophysics and for electrostatic (coulombic) potentials in molecular simulations solves this N-body problem for any given precision with $O(N)$ runtime complexity against $O(N^2)$ for the direct computation.

The potential field is decomposed in a near field part, directly computed, and a far field part approximated thanks to multipole and local expansions. We introduced a matrix formulation of the FMM that exploits the cache hierarchy on a processor through the Basic Linear Algebra Subprograms (BLAS). Moreover, we developed a parallel adaptive version of the FMM algorithm for heterogeneous particle distributions, which is very efficient on parallel clusters of SMP nodes. Finally on such computers, we developed the first hybrid MPI-thread algorithm, which enables to reach better parallel efficiency and better memory scalability. We plan to work on the following points in HiEPACS.

3.4.1. Improvement of calculation efficiency

Nowadays, the high performance computing community is examining alternative architectures that address the limitations of modern cache-based designs. GPU (Graphics Processing Units) and the Cell processor have thus already been used in astrophysics and in molecular dynamics. The Fast Mutipole Method has also been implemented on GPU. We intend to examine the potential of using these forthcoming processors as a building block for high-end parallel computing in N-body calculations. More precisely, we want to take advantage of our specific underlying BLAS routines to obtain an efficient and easily portable FMM for these new architectures. Algorithmic issues such as dynamic load balancing among heterogeneous cores will also have to be solved in order to gather all the available computation power. This research action will be conducd on close connection with the activity described in Section 3.2.
3.4.2. Non uniform distributions

In many applications arising from material physics or astrophysics, the distribution of the data is highly non uniform and the data can grow between two time steps. As mentioned previously, we have proposed a hybrid MPI-thread algorithm to exploit the data locality within each node. We plan to further improve the load balancing for highly non uniform particle distributions with small computation grain thanks to dynamic load balancing at the thread level and thanks to a load balancing correction over several simulation time steps at the process level.

3.4.3. Fast multipole method for dislocation operators

The engine that we develop will be extended to new potentials arising from material physics such as those used in dislocation simulations. The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. Several approaches based on the FMM or based on spatial decomposition in boxes are proposed to speed-up the computation. In dislocation codes, the calculation of the interaction forces between dislocations is still the most CPU consuming. This computation has to be improved to obtain faster and more accurate simulations. Moreover, in such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically balance the computational load are crucial to achieve high performance.

3.4.4. Fast multipole method for boundary element methods

The boundary element method (BEM) is a well known solution of boundary value problems appearing in various fields of physics. With this approach, we only have to solve an integral equation on the boundary. This implies an interaction that decreases in space, but results in the solution of a dense linear system with $O(N^3)$ complexity. The FMM calculation that performs the matrix-vector product enables the use of Krylov subspace methods. Based on the parallel data distribution of the underlying octree implemented to perform the FMM, parallel preconditioners can be designed that exploit the local interaction matrices computed at the finest level of the octree. This research action will be conducted on close connection with the activity described in Section 3.3. Following our earlier experience, we plan to first consider approximate inverse preconditioners that can efficiently exploit these data structures.

3.5. Load balancing algorithms for complex simulations

Participants: Aurélien Esnard, Maria Predari, Pierre Ramet, Jean Roman.

Many important physical phenomena in material physics and climatology are inherently complex applications. They often use multi-physics or multi-scale approaches, which couple different models and codes. The key idea is to reuse available legacy codes through a coupling framework instead of merging them into a stand-alone application. There is typically one model per different scale or physics and each model is implemented by a parallel code.

For instance, to model a crack propagation, one uses a molecular dynamic code to represent the atomistic scale and an elasticity code using a finite element method to represent the continuum scale. Indeed, fully microscopic simulations of most domains of interest are not computationally feasible. Combining such different scales or physics is still a challenge to reach high performance and scalability.

Another prominent example is found in the field of aeronautical propulsion: the conjugate heat transfer simulation in complex geometries (as developed by the CFD team of CERFACS) requires to couple a fluid/convection solver (AVBP) with a solid/conduction solver (AVTP). As the AVBP code is much more CPU consuming than the AVTP code, there is an important computational imbalance between the two solvers.
In this context, one crucial issue is undoubtedly the load balancing of the whole coupled simulation that remains an open question. The goal here is to find the best data distribution for the whole coupled simulation and not only for each stand-alone code, as it is most usually done. Indeed, the naïve balancing of each code on its own can lead to an important imbalance and to a communication bottleneck during the coupling phase, which can drastically decrease the overall performance. Therefore, we argue that it is required to model the coupling itself in order to ensure a good scalability, especially when running on massively parallel architectures (tens of thousands of processors/cores). In other words, one must develop new algorithms and software implementation to perform a coupling-aware partitioning of the whole application. Another related problem is the problem of resource allocation. This is particularly important for the global coupling efficiency and scalability, because each code involved in the coupling can be more or less computationally intensive, and there is a good trade-off to find between resources assigned to each code to avoid that one of them waits for the other(s). What does furthermore happen if the load of one code dynamically changes relatively to the other one? In such a case, it could be convenient to dynamically adapt the number of resources used during the execution.

There are several open algorithmic problems that we investigate in the HiEPAcS project-team. All these problems use a similar methodology based upon the graph model and are expressed as variants of the classic graph partitioning problem, using additional constraints or different objectives.

3.5.1. Dynamic load-balancing with variable number of processors

As a preliminary step related to the dynamic load balancing of coupled codes, we focus on the problem of dynamic load balancing of a single parallel code, with variable number of processors. Indeed, if the workload varies drastically during the simulation, the load must be redistributed regularly among the processors. Dynamic load balancing is a well studied subject but most studies are limited to an initially fixed number of processors. Adjusting the number of processors at runtime allows one to preserve the parallel code efficiency or keep running the simulation when the current memory resources are exceeded. We call this problem, MxN graph repartitioning.

We propose some methods based on graph repartitioning in order to re-balance the load while changing the number of processors. These methods are split in two main steps. Firstly, we study the migration phase and we build a “good” migration matrix minimizing several metrics like the migration volume or the number of exchanged messages. Secondly, we use graph partitioning heuristics to compute a new distribution optimizing the migration according to the previous step results.

3.5.2. Load balancing of coupled codes

As stated above, the load balancing of coupled code is a major issue, that determines the performance of the complex simulation, and reaching high performance can be a great challenge. In this context, we develop new graph partitioning techniques, called co-partitioning. They address the problem of load balancing for two coupled codes: the key idea is to perform a “coupling-aware” partitioning, instead of partitioning these codes independently, as it is classically done. More precisely, we propose to enrich the classic graph model with inter-edges, which represent the coupled code interactions. We describe two new algorithms, and compare them to the naïve approach. In the preliminary experiments we perform on synthetically-generated graphs, we notice that our algorithms succeed to balance the computational load in the coupling phase and in some cases they succeed to reduce the coupling communications costs. Surprisingly, we notice that our algorithms do not degrade significantly the global graph edge-cut, despite the additional constraints that they impose.

Besides this, our co-partitioning technique requires to use graph partitioning with fixed vertices, that raises serious issues with state-of-the-art software, that are classically based on the well-known recursive bisection paradigm (RB). Indeed, the RB method often fails to produce partitions of good quality. To overcome this issue, we propose a new direct k-way greedy graph growing algorithm, called KGGGP, that overcomes this issue and succeeds to produce partition with better quality than RB while respecting the constraint of fixed vertices. Experimental results compare KGGGP against state-of-the-art methods, such as Scotch, for real-life graphs available from the popular DIMACS’10 collection.
3.5.3. Load balancing strategies for hybrid sparse linear solvers

Graph handling and partitioning play a central role in the activity described here but also in other numerical techniques detailed in sparse linear algebra Section. The Nested Dissection is now a well-known heuristic for sparse matrix ordering to both reduce the fill-in during numerical factorization and to maximize the number of independent computation tasks. By using the block data structure induced by the partition of separators of the original graph, very efficient parallel block solvers have been designed and implemented according to super-nodal or multi-frontal approaches. Considering hybrid methods mixing both direct and iterative solvers such as HIPS or MaPhyS, obtaining a domain decomposition leading to a good balancing of both the size of domain interiors and the size of interfaces is a key point for load balancing and efficiency in a parallel context. We intend to revisit some well-known graph partitioning techniques in the light of the hybrid solvers and design new algorithms to be tested in the Scotch package.

4. Application Domains

4.1. Material physics

Participants: Pierre Blanchard, Olivier Coulaud, Arnaud Durocher.

Due to the increase of available computer power, new applications in nano science and physics appear such as study of properties of new materials (photovoltaic materials, bio- and environmental sensors, ...), failure in materials, nano-indentation. Chemists, physicists now commonly perform simulations in these fields. These computations simulate systems up to billion of atoms in materials, for large time scales up to several nanoseconds. The larger the simulation, the smaller the computational cost of the potential driving the phenomena, resulting in low precision results. So, if we need to increase the precision, there are two ways to decrease the computational cost. In the first approach, we improve algorithms and their parallelization and in the second way, we will consider a multiscale approach.

A domain of interest is the material aging for the nuclear industry. The materials are exposed to complex conditions due to the combination of thermo-mechanical loading, the effects of irradiation and the harsh operating environment. This operating regime makes experimentation extremely difficult and we must rely on multi-physics and multi-scale modeling for our understanding of how these materials behave in service. This fundamental understanding helps not only to ensure the longevity of existing nuclear reactors, but also to guide the development of new materials for 4th generation reactor programs and dedicated fusion reactors. For the study of crystalline materials, an important tool is dislocation dynamics (DD) modeling. This multiscale simulation method predicts the plastic response of a material from the underlying physics of dislocation motion. DD serves as a crucial link between the scale of molecular dynamics and macroscopic methods based on finite elements; it can be used to accurately describe the interactions of a small handful of dislocations, or equally well to investigate the global behavior of a massive collection of interacting defects.

To explore i.e. to simulate these new areas, we need to develop and/or to improve significantly models, schemes and solvers used in the classical codes. In the project, we want to accelerate algorithms arising in those fields. We will focus on the following topics (in particular in the currently under definition OPTIDIS project in collaboration with CEA Saclay, CEA Ile-de-france and SIMaP Laboratory in Grenoble) in connection with research described at Sections 3.4 and 3.5.

- The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. In dislocation codes, the computation of interaction forces between dislocations is still the most CPU time consuming and has to be improved to obtain faster and more accurate simulations.

- In such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically construct a good load balancing are crucial to achieve high performance.
• From a physical and a simulation point of view, it will be interesting to couple a molecular dynamics model (atomic model) with a dislocation one (mesoscale model). In such three-dimensional coupling, the main difficulties are firstly to find and characterize a dislocation in the atomistic region, secondly to understand how we can transmit with consistency the information between the two micro and meso scales.

4.2. Co-design for scalable numerical algorithms in scientific applications

Participants: Nicolas Bouzat, Mathieu Faverge, Guillaume Latu, Michel Mehrenberger, Pierre Ramet, Jean Roman.

4.2.1. High performance simulation for ITER tokamak

Scientific simulation for ITER tokamak modeling provides a natural bridge between theory and experimentation and is also an essential tool for understanding and predicting plasma behavior. Recent progresses in numerical simulation of fine-scale turbulence and in large-scale dynamics of magnetically confined plasma have been enabled by access to petascale supercomputers. These progresses would have been unreachable without new computational methods and adapted reduced models. In particular, the plasma science community has developed codes for which computer runtime scales quite well with the number of processors up to thousands cores. The research activities of HiePACS concerning the international ITER challenge were involved in the Inria Project Lab C2S@EXA in collaboration with CEA-IRFM and are related to two complementary studies: a first one concerning the turbulence of plasma particles inside a tokamak (in the context of GYSELA code) and a second one concerning the MHD instability edge localized modes (in the context of JOREK code).

Currently, GYSELA is parallelized in an hybrid MPI+OpenMP way and can exploit the power of the current greatest supercomputers. To simulate faithfully the plasma physic, GYSELA handles a huge amount of data and today, the memory consumption is a bottleneck on very large simulations. In this context, mastering the memory consumption of the code becomes critical to consolidate its scalability and to enable the implementation of new numerical and physical features to fully benefit from the extreme scale architectures.

Other numerical simulation tools designed for the ITER challenge aim at making a significant progress in understanding active control methods of plasma edge MHD instability Edge Localized Modes (ELMs) which represent a particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in the tokamak. The goal is to improve the understanding of the related physics and to propose possible new strategies to improve effectiveness of ELM control techniques. The simulation tool used (JOREK code) is related to non linear MHD modeling and is based on a fully implicit time evolution scheme that leads to 3D large very badly conditioned sparse linear systems to be solved at every time step. In this context, the use of PaStiX library to solve efficiently these large sparse problems by a direct method is a challenging issue.

5. Highlights of the Year

5.1. Highlights of the Year

We have presented two approaches using a Block Low-Rank (BLR) compression technique to reduce the memory footprint and/or the time-to-solution of the sparse supernodal solver PaStiX. Thanks to this compression technique, we have been able to solve a 1 billion unknown system (a 3D Laplacian matrix $100 \times 100 \times 100.000$) on a single node with 3Tb of memory. The factorization time for this system was less than 6 hours using 96 cores, and the precision achieved at the first solve was $10^{-5}$. With 10 additional iterative refinement steps, we reached easily $10^{-8}$ in double precision. The cost of one solve was limited to 280 seconds. We were able to save 9Tb over the 11Tb that would be requested by the direct solver. The last release of the software (PaStiX 6.0) includes these implementations and the description of the parameters are documented in solverstack/pastix.
2017 has been the last year of the FASTLA associate team that has been for 6 years the framework of fruitful and intense research collaborations with Lawrence Berkeley National Laboratory and Stanford University on data sparse numerical algorithms; the joint research addressed especially fast multipole techniques and low rank calculation in sparse linear algebra. This successful collaboration has been concluded by the participation of E. Ng, head of Applied Mathematics Department at Berkeley, to the two HDR juries of A. Guermouche and P. Ramet that have been defended on the same day, November 27th.

6. New Software and Platforms

6.1. Chameleon

**KEYWORDS**: Runtime system - Task-based algorithm - Dense linear algebra - HPC - Task scheduling

**SCIENTIFIC DESCRIPTION**: Chameleon is part of the MORSE (Matrices Over Runtime Systems @ Exascale) project. The overall objective is to develop robust linear algebra libraries relying on innovative runtime systems that can fully benefit from the potential of those future large-scale complex machines.

We expect advances in three directions based first on strong and closed interactions between the runtime and numerical linear algebra communities. This initial activity will then naturally expand to more focused but still joint research in both fields.

1. Fine interaction between linear algebra and runtime systems. On parallel machines, HPC applications need to take care of data movement and consistency, which can be either explicitly managed at the level of the application itself or delegated to a runtime system. We adopt the latter approach in order to better keep up with hardware trends whose complexity is growing exponentially. One major task in this project is to define a proper interface between HPC applications and runtime systems in order to maximize productivity and expressivity. As mentioned in the next section, a widely used approach consists in abstracting the application as a DAG that the runtime system is in charge of scheduling. Scheduling such a DAG over a set of heterogeneous processing units introduces a lot of new challenges, such as predicting accurately the execution time of each type of task over each kind of unit, minimizing data transfers between memory banks, performing data prefetching, etc.

Expected advances: In a nutshell, a new runtime system API will be designed to allow applications to provide scheduling hints to the runtime system and to get real-time feedback about the consequences of scheduling decisions.

2. Runtime systems. A runtime environment is an intermediate layer between the system and the application. It provides low-level functionality not provided by the system (such as scheduling or management of the heterogeneity) and high-level features (such as performance portability). In the framework of this proposal, we will work on the scalability of runtime environment. To achieve scalability it is required to avoid all centralization. Here, the main problem is the scheduling of the tasks. In many task-based runtime environments the scheduler is centralized and becomes a bottleneck as soon as too many cores are involved. It is therefore required to distribute the scheduling decision or to compute a data distribution that imposes the mapping of task using, for instance the so-called “owner-compute” rule. Expected advances: We will design runtime systems that enable an efficient and scalable use of thousands of distributed multicore nodes enhanced with accelerators.

3. Linear algebra. Because of its central position in HPC and of the well understood structure of its algorithms, dense linear algebra has often pioneered new challenges that HPC had to face. Again, dense linear algebra has been in the vanguard of the new era of petascale computing with the design of new algorithms that can efficiently run on a multicore node with GPU accelerators. These algorithms are called “communication-avoiding” since they have been redesigned to limit the amount of communication between processing units (and between the different levels of memory hierarchy). They are expressed through Direct Acyclic Graphs (DAG) of fine-grained tasks that are dynamically scheduled. Expected advances: First, we plan to investigate the impact of these principles in the case of sparse applications (whose algorithms are slightly more complicated but often rely on dense kernels). Furthermore, both in the dense and sparse cases, the scalability on thousands of nodes is still limited, new numerical approaches need to be found. We will specifically design sparse hybrid direct/iterative methods that represent a promising approach.
Overall end point. The overall goal of the MORSE associate team is to enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

**FUNCTIONAL DESCRIPTION:** Chameleon is a dense linear algebra software relying on sequential task-based algorithms where sub-tasks of the overall algorithms are submitted to a Runtime system. A Runtime system such as StarPU is able to manage automatically data transfers between not shared memory area (CPUs-GPUs, distributed nodes). This kind of implementation paradigm allows to design high performing linear algebra algorithms on very different type of architecture: laptop, many-core nodes, CPUs-GPUs, multiple nodes. For example, Chameleon is able to perform a Cholesky factorization (double-precision) at 80 TFlop/s on a dense matrix of order 400 000 (e.i. 4 min).

**RELEASE FUNCTIONAL DESCRIPTION:** Chameleon includes the following features:
- BLAS 3, LAPACK one-sided and LAPACK norms tile algorithms - Support QUARK and StarPU runtime systems - Exploitation of homogeneous and heterogeneous platforms through the use of BLAS/LAPACK CPU kernels and cuBLAS/MAGMA CUDA kernels - Exploitation of clusters of interconnected nodes with distributed memory (using OpenMPI)

- Participants: Cédric Castagnede, Samuel Thibault, Emmanuel Agullo, Florent Pruvost and Mathieu Faverge
- Partners: Innovative Computing Laboratory (ICL) - King Abdullah University of Science and Technology - University of Colorado Denver
- Contact: Emmanuel Agullo
- URL: [https://project.inria.fr/chameleon/](https://project.inria.fr/chameleon/)

### 6.2. Fabulous

**Fast Accurate Block Linear krylov Solver**

**KEYWORDS:** Numerical algorithm - Block Krylov solver

**SCIENTIFIC DESCRIPTION:** Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides

**FUNCTIONAL DESCRIPTION:** Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides. The library implements block variants of minimal norm residual variants with partial convergence management and spectral information recycling. The package already implements regular block-GMRES (BGMRES), Inexact Breakdown BGMRES (IB-BGMRES), Inexact Breakdown BGMRES with Deflated Restarting (IB-BGMRES-DR), Block Generalized Conjugate Residual with partial convergence management. The C++ library relies on callback mechanisms to implement the calculations (matrix-vector, dot-product, ...) that depend on the parallel data distribution selected by the user.

- Participants: Emmanuel Agullo, Luc Giraud and Cyrille Piacibello
- Contact: Luc Giraud
- Publication: Block GMRES method with inexact breakdowns and deflated restarting
- URL: [https://gitlab.inria.fr/solverstack/fabulous/](https://gitlab.inria.fr/solverstack/fabulous/)

### 6.3. HIPS

**Hierarchical Iterative Parallel Solver**

**KEYWORDS:** Simulation - HPC - Parallel calculation - Hybrid direct iterative method
**Scientific Description:** The key point of the methods implemented in HIPS is to define an ordering and a partition of the unknowns that relies on a form of nested dissection ordering in which cross points in the separators play a special role (Hierarchical Interface Decomposition ordering). The subgraphs obtained by nested dissection correspond to the unknowns that are eliminated using a direct method and the Schur complement system on the remaining of the unknowns (that correspond to the interface between the subgraphs viewed as sub-domains) is solved using an iterative method (GMRES or Conjugate Gradient at the time being). This special ordering and partitioning allows for the use of dense block algorithms both in the direct and iterative part of the solver and provides a high degree of parallelism to these algorithms. The code provides a hybrid method which blends direct and iterative solvers. HIPS exploits the partitioning and multistage ILU techniques to enable a highly parallel scheme where several subdomains can be assigned to the same process. It also provides a scalar preconditioner based on the multistage ILUT factorization.

HIPS can be used as a standalone program that reads a sparse linear system from a file, it also provides an interface to be called from any C, C++ or Fortran code. It handles symmetric, unsymmetric, real or complex matrices. Thus, HIPS is a software library that provides several methods to build an efficient preconditioner in almost all situations.

**Functional Description:** HIPS (Hierarchical Iterative Parallel Solver) is a scientific library that provides an efficient parallel iterative solver for very large sparse linear systems.

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- **Contact:** Pierre Ramet
- **URL:** [http://hips.gforge.inria.fr/](http://hips.gforge.inria.fr/)

### 6.4. MAPHYS

**Massively Parallel Hybrid Solver**

**Keyword:** Parallel hybrid direct/iterative solution of large linear systems

**Functional Description:** MaPHyS is a software package that implements a parallel linear solver coupling direct and iterative approaches. The underlying idea is to apply to general unstructured linear systems domain decomposition ideas developed for the solution of linear systems arising from PDEs. The interface problem, associated with the so called Schur complement system, is solved using a block preconditioner with overlap between the blocks that is referred to as Algebraic Additive Schwarz. A fully algebraic coarse space is available for symmetric positive definite problems, that insures the numerical scalability of the preconditioner.

The parallel implementation is based on MPI+thread. Maphys relies on state-of-the-art sparse and dense direct solvers.

MaPHyS is essentially a preconditioner that can be used to speed-up the convergence of any Krylov subspace method and is coupled with the ones implemented in the Fabulous package.

- **Participants:** Emmanuel Agullo, Luc Giraud, Matthieu Kuhn, Gilles Marait and Louis Poirel
- **Contact:** Emmanuel Agullo
- **Publications:** Hierarchical hybrid sparse linear solver for multicore platforms, Robust coarse spaces for Abstract Schwarz preconditioners via generalized eigenproblems
- **URL:** [https://gitlab.inria.fr/solverstack/maphys](https://gitlab.inria.fr/solverstack/maphys)

### 6.5. MetaPart

**Keywords:** High performance computing - HPC - Parallel computing - Graph algorithmics - Graph - Hypergraph
FUNCTIONAL DESCRIPTION: MetaPart is a framework for graph or hypergraph manipulation that addresses different problems, like partitioning, repartitioning, or co-partitioning, ... MetaPart is made up of several projects, such as StarPart, LibGraph or CoPart. StarPart is the core of the MetaPart framework. It offers a wide variety of graph partitioning methods (Metis, Scotch, Zoltan, Patoh, ParMetis, Kahip, ...), which makes it easy to compare these different methods and to better adjust the parameters of these methods. It is built upon the LibGraph library, that provides basic graph & hypergraph routines. The Copart project is a library used on top of StarPart, that provides co-partitioning algorithms for the load-blancing of parallel coupled simulations.

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6.6. MPICPL

MPI CouPLing

KEYWORDS: MPI - Coupling software

FUNCTIONAL DESCRIPTION: MPICPL is a software library dedicated to the coupling of parallel legacy codes, that are based on the well-known MPI standard. It proposes a lightweight and comprehensive programing interface that simplifies the coupling of several MPI codes (2, 3 or more). MPICPL facilitates the deployment of these codes thanks to the mpicplrun tool and it interconnects them automatically through standard MPI inter-communicators. Moreover, it generates the universe communicator, that merges the world communicators of all coupled-codes. The coupling infrastructure is described by a simple XML file, that is just loaded by the mpicplrun tool.

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6.7. OptiDis

KEYWORDS: Dislocation dynamics simulation - Fast multipole method - Large scale - Collision

FUNCTIONAL DESCRIPTION: OptiDis is a new code for large scale dislocation dynamics simulations. Its purpose is to simulate real life dislocation densities (up to 5,1022 dislocations/m-2) in order to understand plastic deformation and study strain hardening. The main application is to observe and understand plastic deformation of irradiated zirconium. Zirconium alloys are the first containment barrier against the dissemination of radioactive elements. More precisely, with neutron irradiated zirconium alloys we are talking about channeling mechanism, which means to stick with the reality, more than tens of thousands of induced loops, i. e. 100 million degrees of freedom in the simulation. The code is based on Numodis code developed at CEA Saclay and the ScalFMM library developed in H/14iePACS project. The code is written in C++ language and using the last features of C++11. One of the main aspects is the hybrid parallelism MPI/OpenMP that gives the software the ability to scale on large cluster while the computation load rises. In order to achieve that, we use different levels of parallelism. First of all, the simulation box is distributed over MPI processes, then we use a thinner level for threads, dividing the domain by an Octree representation. All theses parts are controlled by the ScalFMM library. On the last level, our data are stored in an adaptive structure that absorbs the dynamics of this type of simulation and manages the parallelism of tasks.

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6.8. PaStiX

Parallel Sparse matriX package
KEYWORDS: Sparse Matrices - Factorisation - High-performance calculation - Linear algebra - Linear Systems Solver

SCIENTIFIC DESCRIPTION: PaStiX is based on an efficient static scheduling and memory manager, in order to solve 3D problems with more than 50 million of unknowns. The mapping and scheduling algorithm handle a combination of 1D and 2D block distributions. A dynamic scheduling can also be applied to take care of NUMA architectures while taking into account very precisely the computational costs of the BLAS 3 primitives, the communication costs and the cost of local aggregations.

FUNCTIONAL DESCRIPTION: PaStiX is a scientific library that provides a high performance parallel solver for very large sparse linear systems based on block direct and block ILU(k) methods. It can handle low-rank compression techniques to reduce the computation and the memory complexity. Numerical algorithms are implemented in single or double precision (real or complex) for LDLt, LDLt and LU factorization with static pivoting (for non symmetric matrices having a symmetric pattern). The PaStiX library uses the graph partitioning and sparse matrix block ordering packages Scotch or Metis. The PaStiX solver is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of multicore nodes with GPU accelerators or KNL processors. In particular, we provide a high-performance version with a low memory overhead for multicore node architectures, which fully exploits the advantage of shared memory by using an hybrid MPI-thread implementation.

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6.9. ScalFMM

Scalable Fast Multipole Method

KEYWORDS: N-body - Fast multipole method - Parallelism - MPI - OpenMP

SCIENTIFIC DESCRIPTION: ScalFMM is a software library to simulate N-body interactions using the Fast Multipole Method. The library offers two methods to compute interactions between bodies when the potential decays like 1/r. The first method is the classical FMM based on spherical harmonic expansions and the second is the Black-Box method which is an independent kernel formulation (introduced by E. Darve @ Stanford). With this method, we can now easily add new non oscillatory kernels in our library. For the classical method, two approaches are used to decrease the complexity of the operators. We consider either matrix formulation that allows us to use BLAS routines or rotation matrix to speed up the M2L operator.

ScalFMM intends to offer all the functionalities needed to perform large parallel simulations while enabling an easy customization of the simulation components: kernels, particles and cells. It works in parallel in a shared/distributed memory model using OpenMP and MPI. The software architecture has been designed with two major objectives: being easy to maintain and easy to understand. There is two main parts:

- the management of the octree and the parallelization of the method the kernels. This new architecture allow us to easily add new FMM algorithm or kernels and new paradigm of parallelization.
- the communication components: message passing and synchronization.

FUNCTIONAL DESCRIPTION: Compute N-body interactions using the Fast Multipole Method for large number of objects

- Participants: Bramas Bérenger and Olivier Coulaud
- Contact: Olivier Coulaud
- URL: https://gitlab.inria.fr/solverstack/ScalFMM

6.10. VITE

Visual Trace Explorer

KEYWORDS: Visualization - Execution trace
**FUNCTIONAL DESCRIPTION:** ViTE is a trace explorer. It is a tool made to visualize execution traces of large parallel programs. It supports Pajé, a trace format created by Inria Grenoble, and OTF and OTF2 formats, developed by the University of Dresden and allows the programmer a simpler way to analyse, debug and/or profile large parallel applications.

- Participant: Mathieu Faverge
- Contact: Mathieu Faverge
- URL: http://vite.gforge.inria.fr/

### 6.11. PlaFRIM

*Plateforme Fédérative pour la Recherche en Informatique et Mathématiques*

**FUNCTIONAL DESCRIPTION:** PlaFRIM is an experimental platform for research in modeling, simulations and high performance computing. This platform has been set up from 2009 under the leadership of Inria Bordeaux Sud-Ouest in collaboration with computer science and mathematics laboratories, respectively Labri and IMB with a strong support in the region Aquitaine.

It aggregates different kinds of computational resources for research and development purposes. The latest technologies in terms of processors, memories and architecture are added when they are available on the market. It is now more than 1,000 cores (excluding GPU and Xeon Phi) that are available for all research teams of Inria Bordeaux, Labri and IMB. This computer is in particular used by all the engineers who work in HiePACS and are advised by F. Rue from the SED.

- Contact: Olivier Coulaud
- URL: https://www.plafrim.fr/en/home/

### 7. New Results

#### 7.1. High-performance computing on next generation architectures

##### 7.1.1. Bridging the gap between OpenMP and task-based runtime systems

With the advent of complex modern architectures, the low-level paradigms long considered sufficient to build High Performance Computing (HPC) numerical codes have met their limits. Achieving efficiency, ensuring portability, while preserving programming tractability on such hardware prompted the HPC community to design new, higher level paradigms while relying on runtime systems to maintain performance. However, the common weakness of these projects is to deeply tie applications to specific expert-only runtime system APIs. The OpenMP specification, which aims at providing common parallel programming means for shared-memory platforms, appears as a good candidate to address this issue thanks to the latest task-based constructs introduced in its revision 4.0. The goal of this paper is to assess the effectiveness and limits of this support for designing a high-performance numerical library, ScalFMM, implementing the fast multipole method (FMM) that we have deeply redesigned with respect to the most advanced features provided by OpenMP 4. We show that OpenMP 4 allows for significant performance improvements over previous OpenMP revisions on recent multicore processors and that extensions to the 4.0 standard allow for strongly improving the performance, bridging the gap with the very high performance that was so far reserved to expert-only runtime system APIs. More details on this work can be found in [17].
7.1.2. Modeling Irregular Kernels of Task-based codes: Illustration with the Fast Multipole Method

The significant increase of the hardware complexity that occurred in the last few years led the high performance community to design many scientific libraries according to a task-based parallelization. The modeling of the performance of the individual tasks (or kernels) they are composed of is crucial for facing multiple challenges as diverse as performing accurate performance predictions, designing robust scheduling algorithms, tuning the applications, etc. Fine-grain modeling such as emulation and cycle-accurate simulation may lead to very accurate results. However, not only their high cost may be prohibitive but they furthermore require a high fidelity modeling of the processor, which makes them hard to deploy in practice. In this paper, we propose an alternative coarse-grain, empirical methodology oblivious to both the target code and the hardware architecture, which leads to robust and accurate timing predictions. We illustrate our approach with a task-based Fast Multipole Method (FMM) algorithm, whose kernels are highly irregular, implemented in the ScalFMM library on top of the StarPU task-based runtime system and the simgrid simulator. More details on this work can be found in [41].

7.1.3. Task-based fast multipole method for clusters of multicore processors

Most high-performance, scientific libraries have adopted hybrid parallelization schemes - such as the popular MPI+OpenMP hybridization - to benefit from the capacities of modern distributed-memory machines. While these approaches have shown to achieve high performance, they require a lot of effort to design and maintain sophisticated synchronization/communication strategies. On the other hand, task-based programming paradigms aim at delegating this burden to a runtime system for maximizing productivity. In this article, we assess the potential of task-based fast multipole methods (FMM) on clusters of multicore processors. We propose both a hybrid MPI+task FMM parallelization and a pure task-based parallelization where the MPI communications are implicitly handled by the runtime system. The latter approach yields a very compact code following a sequential task-based programming model. We show that task-based approaches can compete with a hybrid MPI+OpenMP highly optimized code and that furthermore the compact task-based scheme fully matches the performance of the sophisticated, hybrid MPI+task version, ensuring performance while maximizing productivity. We illustrate our discussion with the ScalFMM FMM library and the StarPU runtime system. More details on this work can be found in [40].

7.1.4. Achieving high-performance with a sparse direct solver on Intel KNL

The need for energy-efficient high-end systems has led hardware vendors to design new types of chips for general purpose computing. However, designing or porting a code tailored for these new types of processing units is often considered as a major hurdle for their broad adoption. In this paper, we consider a modern Intel Xeon Phi processor, namely the Intel Knights Landing (KNL) and a numerical code initially designed for a classical multi-core system. More precisely, we consider the qr_mumps scientific library implementing a sparse direct method on top of the StarPU runtime system. We show that with a portable programming model (task-based programming), a good software support (a robust runtime system coupled with an efficient scheduler) and some well defined hardware and software settings, we are able to transparently run the exact same numerical code. This code not only achieves very high performance (up to 1 TFlop/s) on the KNL but also significantly outperforms a modern Intel Xeon multi-core processor both in terms of time to solution and energy efficiency up to a factor of 2.0. More details on this work can be found in [42].

7.2. High performance solvers for large linear algebra problems

7.2.1. Blocking strategy optimizations for sparse direct linear solver on heterogeneous architectures

The preprocessing steps of sparse direct solvers, ordering and block-symbolic factorization, are two major steps that lead to a reduced amount of computation and memory and to a better task granularity to reach a good level of performance when using BLAS kernels. With the advent of GPUs, the granularity of the block computation became more important than ever. In this paper, we present a reordering strategy that increases
this block granularity. This strategy relies on the block-symbolic factorization to refine the ordering produced by tools such as METIS or Scotch, but it does not impact the number of operations required to solve the problem. We integrate this algorithm in the PaStiX solver and show an important reduction of the number of off-diagonal blocks on a large spectrum of matrices. This improvement leads to an increase in efficiency of up to 20% on GPUs.

These contributions have been published in SIAM Journal on Matrix Analysis and Applications [22].

7.2.2. Sparse supernodal solver using block low-rank compression

In the context of FASTLA associate team, during the last 4 years, we are collaborating with Eric Darve, professor in the Institute for Computational and Mathematical Engineering and the Mechanical Engineering Department at Stanford, on the design of a new efficient sparse direct solvers. We have been working on applying fast direct solvers for dense matrices to the solution of sparse direct systems. We observed that the extend-add operation (during the sparse factorization) is the most time-consuming step. We have therefore developed a series of algorithms to reduce this computational cost.

We presented two approaches using a Block Low-Rank (BLR) compression technique to reduce the memory footprint and/or the time-to-solution of the sparse supernodal solver PaStiX. This flat, non-hierarchical, compression method allows to take advantage of the low-rank property of the blocks appearing during the factorization of sparse linear systems, which come from the discretization of partial differential equations. The first approach, called Minimal Memory, illustrates the maximum memory gain that can be obtained with the BLR compression method, while the second approach, called Just-In-Time, mainly focuses on reducing the computational complexity and thus the time-to-solution. Singular Value Decomposition (SVD) and Rank-Revealing QR (RRQR), as compression kernels, are both compared in terms of factorization time, memory consumption, as well as numerical properties. Experiments on a single node with 24 threads and 128 GB of memory are performed to evaluate the potential of both strategies. On a set of matrices from real-life problems, we demonstrate a memory footprint reduction of up to 4 times using the Minimal Memory strategy and a computational time speedup of up to 3.5 times with the Just-In-Time strategy. Then, we study the impact of configuration parameters of the BLR solver that allowed us to solve a 3D laplacian of 36 million unknowns a single node, while the full-rank solver stopped at 8 million due to memory limitation.

These contributions have been presented at the PDSEC workshop of IPDPS’17 conference [30] and an extended version has been submitted in Journal of Computational Science [48].

7.2.3. Towards a hierarchial symbol factorization for data sparse direct solvers

Hierarchical algorithms based on low-rank compression techniques have led to fully re-design the methods of solving dense linear systems at the dawn of the twenty-first century, significantly reducing the computational costs. However, their application to the treatment of sparse linear systems remains today a major challenge to which both the community of hierarchical matrices and that of the sparse matrices are tackling. For this purpose, a first class of approach has been developed by the community of hierarchical matrices to exploit the sparse matrix structure. If the strong point of these methods is that the resulting algorithm remains hierarchical, these do not manage exploit some zeros as naturally do sparse solvers. In contrast, the fact that a sparse factorization can be seen as a sequence of smaller, dense operations, the community of hollow treasure has explored this property to introduce hierarchical techniques within these elementary operations. However, the resulting algorithm loses the fundamental property of hierarchical algorithms, since the compression hierarchy is only local. As part of this doctoral, we introduce a new algorithm, performing a sparse hierarchical symbolic factorization that allows to exploit precisely the sparse structure the matrix and its factors while preserving a global hierarchical structure for to ensure effective compression. We have shown experimentally that this new approach allows us to obtain at the same time a reduced number of operations (because of its hierarchical character) and a number of non-zero elements as small as a hollow method (through the use of a symbolic factorization).

This work is developped in the A. Falco PhD thesis, it led to a publication in a national conference [31] and will give rise to a submission in an international journal in 2018.
7.3. High performance fast multipole method for N-body problems

7.3.1. Modeling Irregular Kernels of Task-based codes

The significant increase of the hardware complexity that occurred in the last few years led the high performance community to design many scientific libraries according to a task-based parallelization. The modeling of the performance of the individual tasks (or kernels) they are composed of is crucial for facing multiple challenges as diverse as performing accurate performance predictions, designing robust scheduling algorithms, tuning the applications, etc. Fine-grain modeling such as emulation and cycle-accurate simulation may lead to very accurate results. However, not only their high cost may be prohibitive but they furthermore require a high fidelity modeling of the processor, which makes them hard to deploy in practice. In this paper, we propose an alternative coarse-grain, empirical methodology oblivious to both the target code and the hardware architecture, which leads to robust and accurate timing predictions. We illustrate our approach with a task-based Fast Multipole Method (FMM) algorithm, whose kernels are highly irregular, implemented in the ScalFMM library on top of the starpu task-based runtime system and the simgrid simulator. More details on this work can be found in [41].

7.3.2. Task-based fast multipole method for clusters of multicore processors

Most high-performance, scientific libraries have adopted hybrid parallelization schemes - such as the popular MPI+OpenMP hybridization - to benefit from the capacities of modern distributed-memory machines. While these approaches have shown to achieve high performance, they require a lot of effort to design and maintain sophisticated synchronization/communication strategies. On the other hand, task-based programming paradigms aim at delegating this burden to a runtime system for maximizing productivity. In this article, we assess the potential of task-based fast multipole methods (FMM) on clusters of multicore processors. We propose both a hybrid MPI+task FMM parallelization and a pure task-based parallelization where the MPI communications are implicitly handled by the runtime system. The latter approach yields a very compact code following a sequential task-based programming model. We show that task-based approaches can compete with a hybrid MPI+OpenMP highly optimized code and that furthermore the compact task-based scheme fully matches the performance of the sophisticated, hybrid MPI+task version, ensuring performance while maximizing productivity. We illustrate our discussion with the ScalFMM FMM library and the StarPU runtime system. More details on this work can be found in [40].

7.4. Efficient algorithmic for load balancing and code coupling in complex simulations

7.4.1. Comparison of initial partitioning methods for multilevel direct k-way graph partitioning with fixed vertices

In scientific computing, load balancing is a crucial step conditioning the performance of large-scale applications. In this case, an efficient decomposition of the workload to a number of processors is highly necessary. A common approach to solve this problem is to use graph representation and perform a graph partitioning in k parts using the multilevel framework and the recursive bisection (RB) paradigm. However, in graph instances where fixed vertices are used to model additional constraints, RB often produces partitions of poor quality. In this paper, we investigate the difficulties of RB to handle fixed vertices and we compare its results with two different alternatives. The first one, called KGGGP is a direct k-way greedy graph growing partitioning that properly handles fixed vertices while the second one, introduced in kPaToH, uses RB and a post-processing technique to correct the obtained partition. Finally, experimental results on graphs that represent real-life numerical simulations show that both alternative methods provide improved partitions compared to RB. More details on this work can be found in [23].
7.5. Application Domains

7.5.1. Material physics

7.5.1.1. EigenSolver

The adaptive vibrational configuration interaction algorithm has been introduced as a new method to efficiently reduce the dimension of the set of basis functions used in a vibrational configuration interaction process. It is based on the construction of nested bases for the discretization of the Hamiltonian operator according to a theoretical criterion that ensures the convergence of the method. In the present work, the Hamiltonian is written as a sum of products of operators. The purpose of this paper is to study the properties and outline the performance details of the main steps of the algorithm. New parameters have been incorporated to increase flexibility, and their influence has been thoroughly investigated. The robustness and reliability of the method are demonstrated for the computation of the vibrational spectrum up to 3000 cm\(^{-1}\) of a widely studied 6-atom molecule (acetonitrile). Our results are compared to the most accurate up to date computation; we also give a new reference calculation for future work on this system. The algorithm has also been applied to a more challenging 7-atom molecule (ethylene oxide). The computed spectrum up to 3200 cm\(^{-1}\) is the most accurate computation that exists today on such systems. More details on this work can be found in [43], [21].

7.5.1.2. Dislocation

We have focused on the improvements of the parallel collision detection and of the accuracy in the force field computation in the OPTIDIS code.

- a new collision detection algorithm to reliably handle junction formation for Dislocation Dynamics using hybrid OpenMP + MPI parallelism has been developed. The enhanced precision and reliability of this new algorithm allows the use of larger time-steps for faster simulations. Hierarchical methods for collision detection, as well as hybrid parallelism are also used to improve performance;
- we observed that the force field computation depends on how the traversal of the segments list or boxes in the octree was done. New accurate formulas to remove this issue have been developed and we are implementing them in the code. They will be used in the Fast Multipole Method that we have developed previously.

Finally, a new distributed data structure has been developed to enhance the reliability and modularity of OPTIDIS. The new data structure provides an interface to modify safely and reliably the distributed dislocation mesh in order to enforce data consistency across all computation nodes. This interface also improves code modularity allowing the study of data layout performance without modifying the algorithms.

7.5.2. Co-design for scalable numerical algorithms in scientific applications

7.5.2.1. High performance simulation for ITER tokamak

Concerning the GYSELA global non-linear electrostatic code, the efforts during the period have concentrated on the design of a more efficient parallel gyro-average operator for the deployment of very large (future) GYSELA runs. The main unknown of the computation is a distribution function that represents either the density of the guiding centers, either the density of the particles in a tokamak. The switch between these two representations is done thanks to the gyro-average operator. In the previous version of GYSELA, the computation of this operator was achieved thanks to a Padé approximation. In order to improve the precision of the gyro-averaging, a new parallel version based on an Hermite interpolation has been done (in collaboration with the Inria TONUS project-team and IPP Garching). The integration of this new implementation of the gyro-average operator has been done in GYSELA and the parallel benchmarks have been successful. This work is carried on in the framework of the PhD of Nicolas Bouzat (funded by IPL C2S@EXA) co-advised with Michel Mehrenberger from TONUS project-team and in collaboration with Guillaume Latu from CEA-IRFM. The scientific objectives of this work is first to consolidate the parallel version of the gyro-average operator, in particular by designing a scalable MPI+OpenMP parallel version and using a new communication scheme, and second to design new numerical methods for the gyro-average, source and collision operators to deal with new physics in GYSELA. The objective is to tackle kinetic electron configurations for more realistic complex large simulations.
In the context of the EoCoE project, we have collaborations with CEA-IRFM. First, with G. Latu, we have investigated the potential of using the last release of the PaStiX solver (version 6.0) on Intel KNL architecture, and more especially on the MARCONI machine (one of the PRACE supercomputers at Cineca, Italia). The results obtained on this architecture are really promising since we are able to reach more than 1 Tflops using a single node. Secondly, we also have a collaboration with P. Tamain and G. Giorgani on the TOKAM3X code to analyze the performance of using PaStiX as a preconditioner. Since a distributed memory is required during the simulation, the previous release of PaStiX is then used. Some difficulties regarding the Fortran wrapper and some memory issues should be fixed when we will have reimplemented the MPI interface in the current release.

7.5.2.2. High performance simulation for 3D frequency-domain Maxwell’s equations

We also recently developed a collaboration with NACHOS on the HORSE (High Order solver for Radar cross Section Evaluation) simulation code. The aim was to integrate the PaStiX solver, with low-rank compression technique, in a domain decomposition framework to solve 3D frequency-domain Maxwell’s equations. The results are promising since we were able to reduce by two the factorization and the solve time for each subdomain. And we were also able to reduce by two the memory requirements thanks to our compression techniques. This would allow us to consider larger subdomains with the same memory constraints that currently limit the simulations.

7.5.2.3. High performance simulation for atmospheric chemistry

We worked on the development and tests of the Adaptive Semi-Implicit Scheme (ASIS) solver for the simulation of atmospheric chemistry. To solve the Ordinary Differential Equation systems associated with the time evolution of the species concentrations, ASIS adopts a one step linearized implicit scheme with specific treatments of the Jacobian of the chemical fluxes. It conserves mass and has a time stepping module to control the accuracy of the numerical solution. In 5 idealized box model simulations ASIS gives results similar to the higher order implicit schemes derived from the Rosenbrock’s and Gear’s methods and requires less computation and run time at the moderate precision required for atmospheric applications. When implemented in the MOCAGE CTM and the LMD Mars GCM the ASIS solver performs well and reveals weaknesses and limitations of the original semi-implicit solvers used by these two models. ASIS can be easily adapted to various chemical schemes and further developments are foreseen to increase its computational efficiency, and to include the computation of the 10 concentrations of the species in aqueous phase in addition to gas phase chemistry.

More details on this work can be found in [19].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

Airbus Group Innovations research and development contract:
- Design and implementation of linear algebra kernel for FEM-BEM coupling (A. Falco (PhD); Emmanuel Agullo, Luc Giraud, Guillaume Sylvand).
- Design and implementation of FMM and block Krylov solver for BEM applications. The HiBOX project is led by the SME IMACS and funded by the DGA Rapid programme (C. Piacibello (Engineer), Olivier Coulaud, Luc Giraud).

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

9.1.1.1. SOLHAR: SOLvers for Heterogeneous Architectures over Runtime systems
Participants: Emmanuel Agullo, Mathieu Faverge, Abdou Guermouche, Pierre Ramet, Jean Roman, Guillaume Sylvand.
Grant: ANR-MONU
Dates: 2013 – 2017  
Partners: Inria (REALOPT, STORM Bordeaux Sud-Ouest et ROMA Rhone-Alpes), IRIT/INPT, CEA-CESTA et Airbus Group Innovations.

Overview:
During the last five years, the interest of the scientific computing community towards accelerating devices has been rapidly growing. The reason for this interest lies in the massive computational power delivered by these devices. Several software libraries for dense linear algebra have been produced; the related algorithms are extremely rich in computation and exhibit a very regular pattern of access to data which makes them extremely good candidates for GPU execution. On the contrary, methods for the direct solution of sparse linear systems have irregular, indirect memory access patterns that adversely interact with typical GPU throughput optimizations.

This project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with accelerators. The ultimate aim of this project is to achieve the implementation of a software package providing a solver based on direct methods for sparse linear systems of equations. To date, the approaches proposed to achieve this objective are mostly based on a simple offloading of some computational tasks to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems. The development of a production-quality, sparse direct solver requires a considerable research effort along three distinct axes:

- linear algebra: algorithms have to be adapted or redesigned in order to exhibit properties that make their implementation and execution on heterogeneous computing platforms efficient and reliable. This may require the development of novel methods for defining data access patterns that are more suitable for the dynamic scheduling of computational tasks on processing units with considerably different capabilities as well as techniques for guaranteeing a reliable and robust behavior and accurate solutions. In addition, it will be necessary to develop novel and efficient accelerator implementations of the specific dense linear algebra kernels that are used within sparse, direct solvers;
- runtime systems: tools such as the StarPU runtime system proved to be extremely efficient and robust for the implementation of dense linear algebra algorithms. Sparse linear algebra algorithms, however, are commonly characterized by complicated data access patterns, computational tasks with extremely variable granularity and complex dependencies. Therefore, a substantial research effort is necessary to design and implement features as well as interfaces to comply with the needs formalized by the research activity on direct methods;
- scheduling: executing a heterogeneous workload with complex dependencies on a heterogeneous architecture is a very challenging problem that demands the development of effective scheduling algorithms. These will be confronted with possibly limited views of dependencies among tasks and multiple, and potentially conflicting objectives, such as minimizing the makespan, maximizing the locality of data or, where it applies, minimizing the memory consumption.

Given the wide availability of computing platforms equipped with accelerators and the numerical robustness of direct solution methods for sparse linear systems, it is reasonable to expect that the outcome of this project will have a considerable impact on both academic and industrial scientific computing. This project will moreover provide a substantial contribution to the computational science and high-performance computing communities, as it will deliver an unprecedented example of a complex numerical code whose parallelization completely relies on runtime scheduling systems and which is, therefore, extremely portable, maintainable and evolvable towards future computing architectures.

9.1.1.2. DEDALES: Algebraic and geometric domain decomposition for subsurface/groundwater flows

Participants: Emmanuel Agullo, Mathieu Faverge, Luc Giraud, Louis Poirel.
Grant: ANR-14-CE23-0005
Dates: 2014 – 2018
**Partners:** Inria EPI POMDAP (leader); Université Paris 13 - Laboratoire Analyse, Géométrie et Applications; Maison de la Simulation; Andra.

**Overview:** Project DEDALES aims at developing high performance software for the simulation of two phase flow in porous media. The project will specifically target parallel computers where each node is itself composed of a large number of processing cores, such as are found in new generation many-core architectures. The project will be driven by an application to radioactive waste deep geological disposal. Its main feature is phenomenological complexity: water-gas flow in highly heterogeneous medium, with widely varying space and time scales. The assessment of large scale model is of major importance and issue for this application, and realistic geological models have several million grid cells. Few, if at all, software codes provide the necessary physical features with massively parallel simulation capabilities. The aim of the DEDALES project is to study, and experiment with, new approaches to develop effective simulation tools with the capability to take advantage of modern computer architectures and their hierarchical structure. To achieve this goal, we will explore two complementary software approaches that both match the hierarchical hardware architecture: on the one hand, we will integrate a hybrid parallel linear solver into an existing flow and transport code, and on the other hand, we will explore a two level approach with the outer level using (space time) domain decomposition, parallelized with a distributed memory approach, and the inner level as a subdomain solver that will exploit thread level parallelism. Linear solvers have always been, and will continue to be, at the center of simulation codes. However, parallelizing implicit methods on unstructured meshes, such as are required to accurately represent the fine geological details of the heterogeneous media considered, is notoriously difficult. It has also been suggested that time level parallelism could be a useful avenue to provide an extra degree of parallelism, so as to exploit the very large number of computing elements that will be part of these next generation computers. Project DEDALES will show that space-time DD methods can provide this extra level, and can usefully be combined with parallel linear solvers at the subdomain level. For all tasks, realistic test cases will be used to show the validity and the parallel scalability of the chosen approach. The most demanding models will be at the frontier of what is currently feasible for the size of models.

9.1.1.3. **TECSER: Novel high performance numerical solution techniques for RCS computations**

**Participants:** Emmanuel Agullo, Luc Giraud, Matthieu Kuhn.

**Grant:** ANR-14-ASTRID

**Dates:** 2014 – 2017

**Partners:** Inria EPI NACHOS (leader), Corida, HiePACS; Airbus Group Innovations, Nucletudes.

**Overview:** the objective of the TECSER projet is to develop an innovative high performance numerical methodology for frequency-domain electromagnetics with applications to RCS (Radar Cross Section) calculation of complicated structures. This numerical methodology combines a high order hybridized DG method for the discretization of the frequency-domain Maxwell in heterogeneous media with a BEM (Boundary Element Method) discretization of an integral representation of Maxwell’s equations in order to obtain the most accurate treatment of boundary truncation in the case of theoretically unbounded propagation domain. Besides, scalable hybrid iterative/direct domain decomposition based algorithms are used for the solution of the resulting algebraic system of equations.

9.2. **European Initiatives**

9.2.1. **FP7 & H2020 Projects**

9.2.1.1. **EoCoE**

**Title:** Energy oriented Centre of Excellence for computer applications

**Program:** H2020

**Duration:** October 2015 - October 2018

**Coordinator:** CEA

**Partners:**

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)
Commissariat A.L. Energie Atomique et Aux Energies Alternatives (France)
Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique (France)
Consiglio Nazionale Delle Ricerche (Italy)
The Cyprus Institute (Cyprus)
Agenzia Nazionale Per le Nuove Tecnologie, l’energia E Lo Sviluppo Economico Sostenibile (Italy)
Fraunhofer Gesellschaft Zur Forderung Der Angewandten Forschung Ev (Germany)
Instytut Chemii Bioorganicznej Polskiej Akademii Nauk (Poland)
Forschungszentrum Julich (Germany)
Max Planck Gesellschaft Zur Foerderung Der Wissenschaften E.V. (Germany)
University of Bath (United Kingdom)
Universite Libre de Bruxelles (Belgium)
Università Degli Studi di Trento (Italy)

Inria contact: Michel Kern

The aim of the present proposal is to establish an Energy Oriented Centre of Excellence for computing applications, (EoCoE). EoCoE (pronounce “Echo”) will use the prodigious potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable and low carbon energy supply. To achieve this goal, we believe that the present revolution in hardware technology calls for a similar paradigm change in the way application codes are designed. EoCoE will assist the energy transition via targeted support to four renewable energy pillars: Meteo, Materials, Water and Fusion, each with a heavy reliance on numerical modelling. These four pillars will be anchored within a strong transversal multidisciplinary basis providing high-end expertise in applied mathematics and HPC. EoCoE is structured around a central Franco-German hub coordinating a pan-European network, gathering a total of 8 countries and 23 teams. Its partners are strongly engaged in both the HPC and energy fields; a prerequisite for the long-term sustainability of EoCoE and also ensuring that it is deeply integrated in the overall European strategy for HPC. The primary goal of EoCoE is to create a new, long-lasting and sustainable community around computational energy science. At the same time, EoCoE is committed to deliver high-impact results within the first three years. It will resolve current bottlenecks in application codes, leading to new modelling capabilities and scientific advances among the four user communities; it will develop cutting-edge mathematical and numerical methods, and tools to foster the usage of Exascale computing. Dedicated services for laboratories and industries will be established to leverage this expertise and to foster an ecosystem around HPC for energy. EoCoE will give birth to new collaborations and working methods and will encourage widely spread best practices.

9.2.1.2. HPC4E

Title: HPC for Energy
Programm: H2020
Duration: December 2015 - November 2017
Coordinator: Barcelona Supercomputing Center

Partners:
- Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas-Ciemat (Spain)
- Iberdrola Renovables Energia (Spain)
- Repsol (Spain)
- Total S.A. (France)
- Lancaster University (United Kingdom)
This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO2 emissions, contribution to diversification of energy supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial applications using alternative fuels, which is required to design efficient furnaces, engines, clean burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth’s interior with unprecedented quality.

9.3. International Initiatives

9.3.1. Inria Associate Teams Not Involved in an Inria International Labs

9.3.1.1. FASTLA

Title: Fast and Scalable Hierarchical Algorithms for Computational Linear Algebra
International Partner (Institution - Laboratory - Researcher):
  Stanford (United States) - Institute for Computational and Mathematical Engineering
  ICME - Eric Darve
Start year: 2012
See also: http://people.bordeaux.inria.fr/coulaud/projets/FastLA_Website/

In this project, we propose to study fast and scalable hierarchical numerical kernels and their implementations on heterogeneous manycore platforms for two major computational kernels in intensive challenging applications. Namely, fast multipole methods (FMM) and sparse linear solvers that appear in many intensive numerical simulations in computational sciences. For the solution of large linear systems, the ultimate goal is to design parallel scalable methods that rely on efficient sparse and dense direct methods using H-matrix arithmetic. Finally, the innovative algorithmic design will be essentially focused on heterogeneous manycore platforms by using task based runtime systems. The partners, Inria HiePACS, Lawrence Berkeley Nat. Lab and Stanford University, have strong, complementary and recognized experiences and backgrounds in these fields

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Member of the Conference Program Committees

  SC’17 (E. Agullo, A. Guermousse), ICPP’17 (A. Guermousse), HiPC’17 (A. Guermousse), IEEE PDP’17 (J. Roman), PDSEC’17 (O. Coulaud, L. Giraud).
10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

L. Giraud is member of the editorial board of the SIAM Journal on Matrix Analysis and Applications (SIMAX).

10.1.2.2. Reviewer - Reviewing Activities


10.1.3. Scientific Expertise

- Luc Giraud is member of the board on Modelisation, Simulation and data analysis of the Competitiveness Cluster for Aeronautics, Space and Embedded Systems.
- Pierre Ramet is "Scientific Expert" at the CEA-DAM CESTA since Oct. 2015.
- Jean Roman is member of the “Scientific Board” of the CEA-DAM. As representative of Inria, he is member of the board of ETP4HPC (European Technology Platform for High Performance Computing), of the French Information Group for PRACE, of the Technical Group of GENCI and of the Scientific Advisory Board of the Maison de la Simulation.

10.1.4. Research Administration

- Emmanuel Agullo and Luc Giraud are the scientific correspondents of the European and International partnership for Inria Bordeaux Sud-Ouest.
- Olivier Coulaud is the coordinator of the PLAFRIM platform for Inria Bordeaux Sud-Ouest.
- Jean Roman is a member of the Direction for Science at Inria: he is the Deputy Scientific Director of the Inria research domain entitled Applied Mathematics, Computation and Simulation and is in charge at the national level of the Inria activities concerning High Performance Computing.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

We indicate below the number of hours spent in teaching activities on a yearly basis for each scientific staff member involved.

Undergraduate level/Licence

- A. Esnard: System programming 36h, Computer architecture 40h, Network 23h at Bordeaux University.
- M. Faverge: Programming environment 26h, Numerical algorithmic 30h, C projects 24h at Bordeaux INP (ENSEIRB-MatMeca).
- P. Ramet: System programming 24h, Databases 32h, Object programming 48h, Distributed programming 32h, Cryptography 32h at Bordeaux University.

Post graduate level/Master

- E. Agullo: Operating systems 24h at Bordeaux University; Dense linear algebra kernels 8h, Numerical algorithms 30h at Bordeaux INP (ENSEIRB-MatMeca).
- O. Coulaud: Paradigms for parallel computing 24h, Hierarchical methods 8h at Bordeaux INP (ENSEIRB-MatMeca).
- A. Esnard: Network management 27h, Network security 27h at Bordeaux University; Programming distributed applications 35h at Bordeaux INP (ENSEIRB-MatMeca).
- M. Faverge: System programming 74h, Load balancing and scheduling 13h at Bordeaux INP (ENSEIRB-MatMeca).
He is also in charge of the master 2 internship for the Computer Science department at Bordeaux INP (ENSEIRB-MatMeca).

- L. Giraud: Introduction to intensive computing and related programming tools 20h, INSA Toulouse; Introduction to high performance computing and applications 20h, ISAE; On mathematical tools for numerical simulations 10h, ENSEEIHT Toulouse; Parallel sparse linear algebra 11h at Bordeaux INP (ENSEIRB-MatMeca).

- A. Guermouche: Network management 92h, Network security 64h, Operating system 24h at Bordeaux University.

- P. Ramet: Load balancing and scheduling 13h, Numerical algorithms 30h at Bordeaux INP (ENSEIRB-MatMeca). He also gives classes on Cryptography 30h, Ho Chi Minh City in Vietnam.

- J. Roman: Parallel sparse linear algebra 10h, Algorithmic and parallel algorithms 22h at Bordeaux INP (ENSEIRB-MatMeca).

He is also in charge of the last year “Parallel and Distributed Computing” option at ENSEIRB-MatMeca which is specialized in HPC (methodologies and applications). This is a common training curriculum between Computer Science and MatMeca departments at Bordeaux INP and with Bordeaux University in the context of Computer Science Research Master. It provides a lot of well-trained internship students for Inria projects working on HPC and simulation.

Summer School: on an annual basis, we run a three day advanced training (lecture and hands on) on parallel linear algebra in the framework of the European PRACE PATC (PRACE Advanced Training Centres) initiative. This training has been organized in many places in France and Europe.

### 10.2.2. Supervision

**HdR :** Abdou Guermouche, Towards efficient sparse direct solvers for modern high-performance architectures, Université de Bordeaux, 27 novembre 2017.

**HdR :** Pierre Ramet, Hierarchical matrices, Hybrid methods, Heterogeneous architectures in sparse linear solvers, Université de Bordeaux, 27 novembre 2017.

**PhD in progress :** Nicolas Bouzat; Fine grain algorithms and deployment methods for exascale plasma physic applications ; M.Mehrenberger (TONUS project-team), J.Roman, G. Latu (CEA-IRFM).

**PhD in progress :** Arnaud Durocher; High performance Dislocation Dynamics simulations on heterogeneous computing platforms for the study of creep deformation mechanisms for nuclear applications; O. Coulaud, L. Dupuy (CEA).

**PhD in progress :** Aurélien Falco; Data sparse calculation in FEM/BEM solution; E. Agullo, L. Giraud, G. Sylvand.

**PhD in progress :** Grégoire Pichon; Utilisation de techniques de compression H-matrices pour solveur direct creux parallèle dans le cadre des applications FEM; M. Faverge, P. Ramet.

**PhD in progress :** Louis Poirel; Algebraic coarse space correction for parallel hybrid solvers; E. Agullo, L. Giraud.

### 10.2.3. Juries


11. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


International Conferences with Proceedings


National Conferences with Proceedings


[32] G. PICHON. Utilisation de la compression Block Low-Rank pour accélérer un solveur direct creux supernodal, in "Conférence d’informatique en Parallélisme, Architecture et Système (ComPAS’17)", Sophia Antipolis, France, June 2017, https://hal.inria.fr/hal-01585660.
Conferences without Proceedings


Research Reports


Other Publications

Project-Team LFANT

Lithe and fast algorithmic number theory

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Algorithmics, Computer Algebra and Cryptology
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Project-Team LFANT

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   A4.3.1. - Public key cryptography
   A8.4. - Computer Algebra
   A8.5. - Number theory
   A8.10. - Computer arithmetic

Other Research Topics and Application Domains:
   B6. - IT and telecom
   B9.4.2. - Mathematics

1. Personnel

Research Scientists
   Andreas Enge [Team leader, Inria, Senior Researcher, HDR]
   Fredrik Johansson [Inria, Researcher]
   Aurel Page [Inria, Researcher, from Sep 2017]
   Damien Robert [Inria, Researcher]

Faculty Members
   Karim Belabas [Univ de Bordeaux, Professor]
   Guilhem Castagnos [Univ de Bordeaux, Associate Professor]
   Jean-Paul Cerri [Univ Bordeaux, Associate Professor]
   Henri Cohen [Univ de Bordeaux, Emeritus]
   Jean-Marc Couveignes [Univ Bordeaux, Professor, HDR]

Technical Staff
   Jared Guissmo Asuncion [Inria, until Jun 2017]
   Bill Allombert [CNRS]

PhD Students
   Jared Guissmo Asuncion [Univ de Bordeaux, from Oct 2017]
   Chloé Martindale [Universities Leiden and Bordeaux]
   Emmanouil Tzortzakis [Universities Leiden and Bordeaux]

Visiting Scientist
   Abdoulaye Maiga [Univ. Dakar, Visiting Scientist]

Administrative Assistants
   Anne-Laure Gautier [Inria]
   Nathalie Robin [Inria]

2. Overall Objectives

2.1. Presentation

Algorithmic number theory dates back to the dawn of mathematics itself, cf. Eratosthenes’s sieve to enumerate consecutive prime numbers. With the arrival of computers, previously unsolvable problems have come into reach, which has boosted the development of more or less practical algorithms for essentially all number theoretic problems. The field is now mature enough for a more computer science driven approach, taking into account the theoretical complexities and practical running times of the algorithms.
Concerning the lower level multiprecision arithmetic, folklore has asserted for a long time that asymptotically fast algorithms such as Schönhage–Strassen multiplication are impractical; nowadays, however, they are used routinely. On a higher level, symbolic computation provides numerous asymptotically fast algorithms (such as for the simultaneous evaluation of a polynomial in many arguments or linear algebra on sparse matrices), which have only partially been exploited in computational number theory. Moreover, precise complexity analyses do not always exist, nor do sound studies to choose between different algorithms (an exponential algorithm may be preferable to a polynomial one for a large range of inputs); folklore cannot be trusted in a fast moving area such as computer science.

Another problem is the reliability of the computations; many number theoretic algorithms err with a small probability, depend on unknown constants or rely on a Riemann hypothesis. The correctness of their output can either be ensured by a special design of the algorithm itself (slowing it down) or by an a posteriori verification. Ideally, the algorithm outputs a certificate, providing an independent fast correctness proof. An example is integer factorisation, where factors are hard to obtain but trivial to check; primality proofs have initiated sophisticated generalisations.

One of the long term goals of the LFANT project team is to make an inventory of the major number theoretic algorithms, with an emphasis on algebraic number theory and arithmetic geometry, and to carry out complexity analyses. So far, most of these algorithms have been designed and tested over number fields of small degree and scale badly. A complexity analysis should naturally lead to improvements by identifying bottlenecks, systematically redesigning and incorporating modern asymptotically fast methods.

Reliability of the developed algorithms is a second long term goal of our project team. Short of proving the Riemann hypothesis, this could be achieved through the design of specialised, slower algorithms not relying on any unproven assumptions. We would prefer, however, to augment the fastest unproven algorithms with the creation of independently verifiable certificates. Ideally, it should not take longer to check the certificate than to generate it.

All theoretical results are complemented by concrete reference implementations in PARI/GP, which allow to determine and tune the thresholds where the asymptotic complexity kicks in and help to evaluate practical performances on problem instances provided by the research community. Another important source for algorithmic problems treated by the LFANT project team is modern cryptology. Indeed, the security of all practically relevant public key cryptosystems relies on the difficulty of some number theoretic problem; on the other hand, implementing the systems and finding secure parameters require efficient algorithmic solutions to number theoretic problems.

### 3. Research Program

#### 3.1. Number fields, class groups and other invariants

**Participants:** Bill Allombert, Jared Guissmo Asuncion, Karim Belabas, Jean-Paul Cerri, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Aurel Page.

Modern number theory has been introduced in the second half of the 19th century by Dedekind, Kummer, Kronecker, Weber and others, motivated by Fermat’s conjecture: There is no non-trivial solution in integers to the equation $x^n + y^n = z^n$ for $n \geq 3$. For recent textbooks, see [5]. Kummer’s idea for solving Fermat’s problem was to rewrite the equation as $(x + y)(x + \zeta y)(x + \zeta^2 y) \cdots (x + \zeta^{n-1} y) = z^n$ for a primitive $n$-th root of unity $\zeta$, which seems to imply that each factor on the left hand side is an $n$-th power, from which a contradiction can be derived.

The solution requires to augment the integers by algebraic numbers, that are roots of polynomials in $\mathbb{Z}[X]$. For instance, $\zeta$ is a root of $X^n - 1$, $\sqrt{2}$ is a root of $X^3 - 2$ and $\sqrt[3]{2}$ is a root of $25X^3 - 3$. A number field consists of the rationals to which have been added finitely many algebraic numbers together with their sums, differences, products and quotients. It turns out that actually one generator suffices, and any number field $K$ is isomorphic to $\mathbb{Q}[X]/(f(X))$, where $f(X)$ is the minimal polynomial of the generator. Of special interest
are algebraic integers, “numbers without denominators”, that are roots of a monic polynomial. For instance, \( \sqrt{2} \) and \( \frac{\sqrt{3}}{2} \) are integers, while \( \frac{1}{\sqrt{2}} \) is not. The ring of integers of \( K \) is denoted by \( \mathcal{O}_K \); it plays the same role in \( K \) as \( \mathbb{Z} \) in \( \mathbb{Q} \).

Unfortunately, elements in \( \mathcal{O}_K \) may factor in different ways, which invalidates Kummer’s argumentation. Unique factorisation may be recovered by switching to ideals, subsets of \( \mathcal{O}_K \) that are closed under addition and under multiplication by elements of \( \mathcal{O}_K \). In \( \mathbb{Z} \), for instance, any ideal is principal, that is, generated by one element, so that ideals and numbers are essentially the same. In particular, the unique factorisation of ideals then implies the unique factorisation of numbers. In general, this is not the case, and the class group \( \text{Cl}_K \) of ideals of \( \mathcal{O}_K \) modulo principal ideals and its class number \( h_K = |\text{Cl}_K| \) measure how far \( \mathcal{O}_K \) is from behaving like \( \mathbb{Z} \).

Using ideals introduces the additional difficulty of having to deal with units, the invertible elements of \( \mathcal{O}_K \): Even when \( h_K = 1 \), a factorisation of ideals does not immediately yield a factorisation of numbers, since ideal generators are only defined up to units. For instance, the ideal factorisation \( (6) = (2) \cdot (3) \) corresponds to the two factorisations \( 6 = 2 \cdot 3 \) and \( 6 = (-2) \cdot (-3) \). While in \( \mathbb{Z} \), the only units are 1 and \(-1\), the unit structure in general is that of a finitely generated \( \mathbb{Z} \)-module, whose generators are the fundamental units. The regulator \( R_K \) measures the “size” of the fundamental units as the volume of an associated lattice.

One of the main concerns of algorithmic algebraic number theory is to explicitly compute these invariants (\( \text{Cl}_K \) and \( h_K \), fundamental units and \( R_K \)), as well as to provide the data allowing to efficiently compute with numbers and ideals of \( \mathcal{O}_K \); see [23] for a recent account.

The analytic class number formula links the invariants \( h_K \) and \( R_K \) (unfortunately, only their product) to the \( \zeta \)-function of \( K \), \( \zeta_K(s) := \prod_{\mathfrak{p} \text{ prime ideal of } \mathcal{O}_K} (1 - N\mathfrak{p}^{-s})^{-1} \), which is meaningful when \( \Re(s) > 1 \), but which may be extended to arbitrary complex \( s \neq 1 \). Introducing characters on the class group yields a generalisation of \( \zeta \)-to \( L \)-functions. The generalised Riemann hypothesis (GRH), which remains unproved even over the rationals, states that any such \( L \)-function does not vanish in the right half-plane \( \Re(s) > 1/2 \). The validity of the GRH has a dramatic impact on the performance of number theoretic algorithms. For instance, under GRH, the class group admits a system of generators of polynomial size; without GRH, only exponential bounds are known. Consequently, an algorithm to compute \( \text{Cl}_K \) via generators and relations (currently the only viable practical approach) either has to assume that GRH is true or immediately becomes exponential.

When \( h_K = 1 \) the number field \( K \) may be norm-Euclidean, endowing \( \mathcal{O}_K \) with a Euclidean division algorithm. This question leads to the notions of the Euclidean minimum and spectrum of \( K \), and another task in algorithmic number theory is to explicitly determine this minimum and the upper part of this spectrum, yielding for instance generalised Euclidean gcd algorithms.

### 3.2. Function fields, algebraic curves and cryptology

**Participants:** Karim Belabas, Guilhem Castagnos, Jean-Marc Couveignes, Andreas Enge, Damien Robert, Emmanueln Tzortzakis.

Algebraic curves over finite fields are used to build the currently most competitive public key cryptosystems. Such a curve is given by a bivariate equation \( C(X,Y) = 0 \) with coefficients in a finite field \( \mathbb{F}_q \). The main classes of curves that are interesting from a cryptographic perspective are elliptic curves of equation \( C = Y^2 - (X^3 + aX + b) \) and hyperelliptic curves of equation \( C = Y^2 - (X^{2g+1} + \cdots) \) with \( g \geq 2 \).

The cryptosystem is implemented in an associated finite abelian group, the Jacobian \( \text{Jac}_C \). Using the language of function fields exhibits a close analogy to the number fields discussed in the previous section. Let \( \mathbb{F}_q(X) \) (the analogue of \( \mathbb{Q} \)) be the rational function field with subring \( \mathbb{F}_q[X] \) (which is principal just as \( \mathbb{Z} \)). The function field of \( C \) is \( K_C = \mathbb{F}_q(X)[Y]/(C) \); it contains the coordinate ring \( \mathcal{O}_C = \mathbb{F}_q(X,Y)/(C) \). Definitions and properties carry over from the number field case \( K/Q \) to the function field extension \( K_C/E \). The Jacobian \( \text{Jac}_C \) is the divisor class group of \( K_C \), which is an extension of (and for the curves used in cryptography usually equals) the ideal class group of \( \mathcal{O}_C \).
3.3. Complex multiplication

The size of the Jacobian group, the main security parameter of the cryptosystem, is given by an $L$-function. The GRH for function fields, which has been proved by Weil, yields the Hasse–Weil bound
\[(\sqrt{q} - 1)^{2g} \leq |Jac_C| \leq (\sqrt{q} + 1)^{2g},\]
or $|Jac_C| \approx q^g$, where the genus is an invariant of the curve that correlates with the degree of its equation. For instance, the genus of an elliptic curve is 1, that of a hyperelliptic one is $\frac{deg(X)}{2} - 1$. An important algorithmic question is to compute the exact cardinality of the Jacobian.

The security of the cryptosystem requires more precisely that the discrete logarithm problem (DLP) be difficult in the underlying group; that is, given elements $D_1$ and $D_2 = xD_1$ of $Jac_C$, it must be difficult to determine $x$. Computing $x$ corresponds in fact to computing $Jac_C$ explicitly with an isomorphism to an abstract product of finite cyclic groups; in this sense, the DLP amounts to computing the class group in the function field setting.

For any integer $n$, the Weil pairing $e_n$ on $C$ is a function that takes as input two elements of order $n$ of $Jac_C$ and maps them into the multiplicative group of a finite field extension $\mathbb{F}_q[x]/(x^k - 1)$ depending on $n$. It is bilinear in both its arguments, which allows to transport the DLP from a curve into a finite field, where it is potentially easier to solve. The Tate-Lichtenbaum pairing, that is more difficult to define, but more efficient to implement, has similar properties. From a constructive point of view, the last few years have seen a wealth of cryptosystems with attractive novel properties relying on pairings.

For a random curve, the parameter $k$ usually becomes so big that the result of a pairing cannot even be output any more. One of the major algorithmic problems related to pairings is thus the construction of curves with a given, smallish $k$.

3.3. Complex multiplication

**Participants:** Jared Guissmo Asuncion, Karim Belabas, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Chloë Martindale, Damien Robert.

Complex multiplication provides a link between number fields and algebraic curves; for a concise introduction in the elliptic curve case, see [25], for more background material, [24]. In fact, for most curves $C$ over a finite field, the endomorphism ring of $Jac_C$ is a maximal unramified abelian extension of $K$, called CM field. The CM field of an elliptic curve is an imaginary-quadratic field $\mathbb{Q}(\sqrt{D})$ with $D < 0$, that of a hyperelliptic curve of genus $g$ is an imaginary-quadratic extension of a totally real number field of degree $g$. Deuring’s lifting theorem ensures that $C$ is the reduction modulo some prime of a curve with the same endomorphism ring, but defined over the Hilbert class field $H_K$ of $K$.

Algebraically, $H_K$ is defined as the maximal unramified abelian extension of $K$; the Galois group of $H_K/K$ is then precisely the class group $Cl_K$. A number field extension $H/K$ is called Galois if $H \simeq K[X]/(f)$ and $H$ contains all complex roots of $f$. For instance, $\mathbb{Q}(\sqrt{2})$ is Galois since it contains not only $\sqrt{2}$, but also the second root $-\sqrt{2}$ of $X^2 - 2$, whereas $\mathbb{Q}(\sqrt{2})$ is not Galois, since it does not contain the root $e^{\pi i/3} \sqrt{2}$ of $X^3 - 2$. The Galois group $\text{Gal}_{H/K}$ is the group of automorphisms of $H$ that fix $K$; it permutes the roots of $f$.

Finally, an abelian extension is a Galois extension with abelian Galois group.

Analytically, in the elliptic case $H_K$ may be obtained by adjoining to $K$ the singular value $j(\tau)$ for a complex valued, so-called modular function $j$ in some $\tau \in \mathcal{O}_K$; the correspondence between $\text{Gal}_{H/K}$ and $Cl_K$ allows to obtain the different roots of the minimal polynomial $f$ of $j(\tau)$ and finally $f$ itself. A similar, more involved construction can be used for hyperelliptic curves. This direct application of complex multiplication yields algebraic curves whose $L$-functions are known beforehand; in particular, it is the only possible way of obtaining ordinary curves for pairing-based cryptosystems.

The same theory can be used to develop algorithms that, given an arbitrary curve over a finite field, compute its $L$-function.

A generalisation is provided by ray class fields; these are still abelian, but allow for some well-controlled ramification. The tools for explicitly constructing such class fields are similar to those used for Hilbert class fields.
4. Highlights of the Year

4.1. Highlights of the Year

Aurel Page has been recruited as an Inria CR in the team.
Damien Robert organised a one-week workshop with the members of the associated team FAST with several African countries.
The book [17] by Henri Cohen on *Modular Forms: A Classical Approach* has been published.

4.1.1. Awards

The paper [] describing Arb in the IEEE Transactions on Computers was selected as the best paper of this journal’s Special Issue on Computer Arithmetic.

5. New Software and Platforms

5.1. APIP

*Another Pairing Implementation in PARI*

**Scientific Description:** Apip, Another Pairing Implementation in PARI, is a library for computing standard and optimised variants of most cryptographic pairings.

The following pairings are available: Weil, Tate, ate and twisted ate, optimised versions (à la Vercauteren–Hess) of ate and twisted ate for selected curve families.

The following methods to compute the Miller part are implemented: standard Miller double-and-add method, standard Miller using a non-adjacent form, Boxall et al. version, Boxall et al. version using a non-adjacent form.

The final exponentiation part can be computed using one of the following variants: naive exponentiation, interleaved method, Avanzi–Mihăilescu’s method, Kato et al.’s method, Scott et al.’s method.

Part of the library has been included into Pari/Gp proper.

**Functional Description:** APIP is a library for computing standard and optimised variants of most cryptographic pairings.

- Participant: Jérôme Milan
- Contact: Jérôme Milan
- URL: [http://www.lix.polytechnique.fr/~milanj/apip/apip.xhtml](http://www.lix.polytechnique.fr/~milanj/apip/apip.xhtml)

5.2. AVIsogenies

*Abelian Varieties and Isogenies*

**Functional Description:** AVIsogenies is a Magma package for working with abelian varieties, with a particular emphasis on explicit isogeny computation.

Its prominent feature is the computation of (1,l)-isogenies between Jacobian varieties of genus-two hyperelliptic curves over finite fields of characteristic coprime to l, practical runs have used values of l in the hundreds.

It can also be used to compute endomorphism rings of abelian surfaces, and find complete addition laws on them.

- Participants: Damien Robert, Gaëtan Bisson and Romain Cosset
- Contact: Gaëtan Bisson
- URL: [http://avisogenies.gforge.inria.fr/](http://avisogenies.gforge.inria.fr/)
5.3. CM

**KEYWORD:** Arithmetic

**FUNCTIONAL DESCRIPTION:** The Cm software implements the construction of ring class fields of imaginary quadratic number fields and of elliptic curves with complex multiplication via floating point approximations. It consists of libraries that can be called from within a C program and of executable command line applications.

**RELEASE FUNCTIONAL DESCRIPTION:** Features - Precisions beyond 300000 bits are now supported by an addition chain of variable length for the -function. Dependencies - The minimal version number of Mpf has been increased to 3.0.0, that of Mpc to 1.0.0 and that of Pari to 2.7.0.

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/

5.4. CMH

**Computation of Igusa Class Polynomials**

**KEYWORDS:** Mathematics - Cryptography - Number theory

**FUNCTIONAL DESCRIPTION:** Cmh computes Igusa class polynomials, parameterising two-dimensional abelian varieties (or, equivalently, Jacobians of hyperelliptic curves of genus 2) with given complex multiplication.

- Participants: Andreas Enge, Emmanuel Thomé and Regis Dupont
- Contact: Emmanuel Thomé
- URL: http://cmh.gforge.inria.fr

5.5. CUBIC

**FUNCTIONAL DESCRIPTION:** Cubic is a stand-alone program that prints out generating equations for cubic fields of either signature and bounded discriminant. It depends on the Pari library. The algorithm has quasi-linear time complexity in the size of the output.

- Participant: Karim Belabas
- Contact: Karim Belabas
- URL: http://www.math.u-bordeaux1.fr/~belabas/research/software/cubic-1.2.tgz

5.6. Euclid

**FUNCTIONAL DESCRIPTION:** Euclid is a program to compute the Euclidean minimum of a number field. It is the practical implementation of the algorithm described in [38] . Some corresponding tables built with the algorithm are also available. Euclid is a stand-alone program depending on the PARI library.

- Participants: Jean-Paul Cerri and Pierre Lezowski
- Contact: Pierre Lezowski
- URL: http://www.math.u-bordeaux1.fr/~plezowski/euclid/index.php

5.7. KleinianGroups

**FUNCTIONAL DESCRIPTION:** KleinianGroups is a Magma package that computes fundamental domains of arithmetic Kleinian groups.

- Participant: Aurel Page
- Contact: Aurel Page
5.8. GNU MPC

**Keywords:** Arithmetic

**Functional Description:** Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It is built upon and follows the same principles as Mpfr. The library is written by Andreas Enge, Philippe Théveny and Paul Zimmermann.

**Release Functional Description:** Fixed `mpc_pow`, see http://lists.gforge.inria.fr/pipermail/mpc-discuss/2014-October/001315.html - #18257: Switched to libtool 2.4.5.

- Participants: Andreas Enge, Mickaël Gastineau, Paul Zimmermann and Philippe Théveny
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/

5.9. MPFRCX

**Keywords:** Arithmetic

**Functional Description:** Mpfrcx is a library for the arithmetic of univariate polynomials over arbitrary precision real (Mpfr) or complex (Mpc) numbers, without control on the rounding. For the time being, only the few functions needed to implement the floating point approach to complex multiplication are implemented. On the other hand, these comprise asymptotically fast multiplication routines such as Toom-Cook and the FFT.

**Release Functional Description:** - new function `product_and_hecke`
- improved memory consumption for unbalanced FFT multiplications

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/

5.10. PARI/GP

**Keywords:** Computational number theory

**Functional Description:** Pari/Gp is a widely used computer algebra system designed for fast computations in number theory (factorisation, algebraic number theory, elliptic curves, modular forms ...), but it also contains a large number of other useful functions to compute with mathematical entities such as matrices, polynomials, power series, algebraic numbers, etc., and many transcendental functions.

- Participants: Andreas Enge, Hamish Ivey-Law, Henri Cohen and Karim Belabas
- Partner: CNRS
- Contact: Karim Belabas
- URL: http://pari.math.u-bordeaux.fr/

6. New Results

6.1. Non commutative number theory

**Participant:** Jean Paul Cerri.

Pierre Lezowski has studied in [11], Euclidean properties of matrix algebras. He proved that if \( A \) is a commutative ring and if \( n > 1 \) is an integer, then \( M_n(A) \) is right and left Euclidean if and only if \( A \) is a principal ideal ring. Moreover, under the hypothesis that the statham takes integer values, he established that if \( A \) is an integral domain, then \( M_n(A) \) is \( \omega \)-stage right and left Euclidean if and only if \( A \) is a Bézout ring. He also proved, under the same hypothesis, that if \( A \) is a \( K \)-Hermite ring, then \( M_n(A) \) is \((4n - 3)\)-stage left and right Euclidean, that if \( A \) is an elementary divisor ring, then \( M_n(A) \) is \((2n - 1)\)-stage left and right Euclidean, and that if \( A \) is a principal ideal ring, then \( M_n(A) \) is 2-stage right and left Euclidean. In each case, he obtained an explicit algorithm allowing to compute, among other things, right or left gcd in \( M_n(A) \).
Jean-Paul Cerri and Pierre Lezowski have generalized in [18], Cerri’s algorithm (for the computation of the upper part of the norm-Euclidean spectrum of a number field) to totally definite quaternion fields. This allowed them to establish the exact value of the norm-Euclidean minimum of many orders in totally definite quaternion fields over a quadratic number field. Before this work, nobody knew how to compute the exact value of such a minimum when the base number field has degree $d > 1$. They also proved that the Euclidean minimum and the inhomogeneous minimum of orders in such quaternion fields are always equal and that moreover they are rational under the hypothesis that the base number field is not quadratic, which remains the only open case, as for real number fields.

In [12] Lezowski determines which cyclic field of degree $d$ are norm-Euclidean for $d = 5, 7, 19, 31, 37, 47, 59, 67, 71, 73, 79, 97$.

### 6.2. Cryptographic Protocols

**Participant:** Guilhem Castagnos.

In [15] G. Castagnos, L. Imbert, and F. Laguillaumie revisit a recent cryptographic primitive called encryption switching protocols (ESP). This primitive was introduced by Couteau, Peters and Pointcheval last year. It allows to switch ciphertexts between two encryption schemes. If such an ESP is built with two schemes that are respectively additively and multiplicatively homomorphic, it naturally gives rise to a secure 2-party computation protocol. It is thus perfectly suited for evaluating functions, such as multivariate polynomials, given as arithmetic circuits. Couteau et al. built an ESP to switch between Elgamal and Paillier encryptions which do not naturally fit well together. Consequently, they had to design a clever variant of Elgamal over $\mathbb{Z}/n\mathbb{Z}$ with a costly shared decryption.

In this work, Castagnos et. al. first present a conceptually simple generic construction for encryption switching protocols. Then, they give an efficient instantiation of our generic approach that uses two well-suited protocols, namely a variant of Elgamal in $\mathbb{Z}/p\mathbb{Z}$ and the Castagnos-Laguillaumie encryption which is additively homomorphic over $\mathbb{Z}/p\mathbb{Z}$. Among other advantages, this allows to perform all computations modulo a prime $p$ instead of an RSA modulus. Overall, this solution leads to significant reductions in the number of rounds as well as the number of bits exchanged by the parties during the interactive protocols. They also show how to extend its security to the malicious setting.

This paper was presented at the CRYPTO Conference 2017, and is part of the ALAMBIC project.

### 6.3. Algorithmic number theory

**Participant:** Henri Cohen.

The book [17] by Henri Cohen on *Modular Forms: A Classical Approach* has been published. The theory of modular forms is a fundamental tool used in many areas of mathematics and physics. It is also a very concrete subject in itself and abounds with an amazing number of surprising identities. This comprehensive textbook, gives a complete picture of the classical aspects of the subject, with an emphasis on explicit formulas. Content include: elliptic functions and theta functions, the modular group, its subgroups, and general aspects of holomorphic and nonholomorphic modular forms, with an emphasis on explicit examples. The heart of the book is the classical theory developed by Hecke and continued up to the Atkin–Lehner–Li theory of newforms and including the theory of Eisenstein series, Rankin–Selberg theory, and a more general theory of theta series including the Weil representation. The final chapter also explores in some detail more general types of modular forms such as half-integral weight, Hilbert, Jacobi, Maass, and Siegel modular forms.

The article by Bill Allombert, Jean-Paul Allouche and Michel Mendès France on *Euler’s divergent series and an elementary model in Statistical Physics* has been published in Statistical Physics Ars Mathematica Contemporanea. This article study the multiple integral of a multivariate exponential taken with respect either to the Lebesgue measure or to the discrete uniform Bernoulli measure. In the first case the integral is linked to Euler’s everywhere divergent power series and its generalizations, while in the second case the integral is linked to a one-dimensional model of spin systems as encountered in physics.
Bill Allombert has worked with Nicolas Brisebarre and Alain Lasjaunias on a two-valued sequence and related continued fractions in power series fields. They explicitly describe a noteworthy transcendental continued fraction in the field of power series over $\mathbb{Q}$, having irrationality measure equal to $3$. This continued fraction is a generating function of a particular sequence in the set $\{1, 2\}$.

In the Pari software, K. Belabas and H. Cohen have added an extensive new package $\mathbf{mf}$ for modular forms. This package allows to build spaces of classical modular form $M_k(\Gamma_0(N), \chi)$ where $2k \in \mathbb{Z}$ and perform standard tasks like finding bases, splitting the space using Hecke operators and the computation of eigenforms. It also solves important difficult problems: the computation of forms of weight $1$, the realization of Shimura lifts as an explicit isomorphism between Kohnen’s $+\$-space $S^+_k(\Gamma_0(4N), \chi)$ and $S^+_k(\Gamma_0(N), \chi^2)$ and the Fourier expansion of $f \mid_k \gamma$ for arbitrary $f$ and arbitrary $\gamma \in \text{GL}_2(\mathbb{Q})^+$, which includes as a special case the expansion of $f$ at all cusps (where other modular form packages usually deal with the expansion at infinity and the cusps reachable via Atkin-Lehner operators, e.g. all cusps in squarefree levels). The latter is especially important as it allows an explicit description of Atkin-Lehner operators, the evaluation of $f$ at arbitrary points in the upper-half plane, the computation of period polynomials and Pettersson products, etc.

### 6.4. Elliptic curve and Abelian varieties cryptology

**Participant:** Damien Robert.

In [21], E. Milio and D. Robert describe an algorithm to evaluate in quasi-linear time Hilbert modular functions in dimension $2$, and also how to recover in time quasi-linear the period matrix from the value of the function. They apply this theory to the modular functions $j(\tau/\beta)$ and $\theta(\tau/\beta)$ where $\beta$ is a totally real positive number of the quadratic real field corresponding to the Hilbert surface to construct modular polynomials parametrizing cyclic isogenies between principally polarised abelian varieties. This extends the construction of classical modular polynomials but allow to have much smaller polynomials, which allow to compute them up to norm $\ell = 91$ rather than $\ell = 7$ in dimension $2$ for classical polynomials.

In [19], Dudeanu, Alina and Jetchev, Dimitar and Robert, Damien and Vuille, Marius describe an algorithm to compute cyclic isogenies from their kernels. This extends the work of [10] from isogenies with maximal isotropic kernels for the Weil pairing to cyclic isogenies, using real multiplication. Such isogenies are indispensable to fully explore the isogeny graph and will be able to speed up a lot of algorithms that needs isogenous curves, like the CRT method for class polynomials.

### 6.5. Arbitrary-precision ball arithmetic

**Participant:** Fredrik Johansson.

During the year, F. Johansson has released three new versions (2.10, 2.11 and 2.12) of the Arb software for arbitrary-precision ball arithmetic.

The paper [1] describing Arb has been published in the IEEE Transactions on Computers and was selected as the best paper of this journal’s Special Issue on Computer Arithmetic. As a result, a video presentation was featured on the journal’s website and Johansson was invited to present the paper in a special session at the 24th IEEE Symposium on Computer Arithmetic (ARITH24) at Imperial College London, UK.

In [20], Johansson describes the first complete algorithm for computing the Lambert W function rigorously in complex ball arithmetic.

### 6.6. Python and Julia computer algebra packages

**Participant:** Fredrik Johansson.

F. Johansson together with C. Fieker, W. Hart and T. Hofmann of TU Kaiserslautern have developed Nemo and Hecke, two packages for computer algebra and algebraic number theory using the Julia programming language. The paper [16] describing Nemo and Hecke has been published in the proceedings of ISSAC, the main international computer algebra conference.
The paper [14] describing the SymPy package for computer algebra in Python has been published. SymPy is a highly collaborative international project and F. Johansson is one of the 27 coauthors of this paper. Johansson’s main contributions to the software include developing the mpmath package used for arbitrary-precision numerical evaluation. In addition, Johansson has issued the stable version 1.0 release of mpmath.

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. ANR Alambic – AppLicAtions of MalleABIlity in Cryptography

Participant: Guilhem Castagnos.

https://crypto.di.ens.fr/projects:alambic:main

The ALAMBIC project is a research project formed by members of the Inria Project-Team CASCADE of ENS Paris, members of the AriC Inria project-team of ENS Lyon, and members of the CRYPTIS of the university of Limoges. G. Castagnos is an external member of the team of Lyon for this project.

Non-malleability is a security notion for public key cryptographic encryption schemes that ensures that it is infeasible for an adversary to modify ciphertexts into other ciphertexts of messages which are related to the decryption of the first ones. On the other hand, it has been realized that, in specific settings, malleability in cryptographic protocols can actually be a very useful feature. For example, the notion of homomorphic encryption allows specific types of computations to be carried out on ciphertexts and generate an encrypted result which, when decrypted, matches the result of operations performed on the plaintexts. The homomorphic property can be used to create secure voting systems, collision-resistant hash functions, private information retrieval schemes, and for fully homomorphic encryption enables widespread use of cloud computing by ensuring the confidentiality of processed data.

The aim of the ALAMBIC project to investigate further theoretical and practical applications of malleability in cryptography. More precisely, this project focuses on three different aspects: secure computation outsourcing and server-aided cryptography, homomorphic encryption and applications and << paradoxical >> applications of malleability.

7.2. European Initiatives

7.2.1. FP7 & H2020 Projects

Title: OpenDreamKit
Program: H2020
Duration: January 2016 - December 2020
Coordinator: Nicolas Thiéry
Inria contact: Karim Belabas

OpenDreamKit is a Horizon 2020 European Research Infrastructure project (#676541) that will run for four years, starting from September 2015. It provides substantial funding to the open source computational mathematics ecosystem, and in particular popular tools such as LinBox, MPIR, SageMath, GAP, Pari/GP, LMFDB, Singular, MathHub, and the IPython/Jupyter interactive computing environment.

7.3. International Initiatives

7.3.1. Inria International Labs

7.3.1.1. FAST
Title: (Harder Better) FAster STronger cryptography

International Partner

Université des Sciences et Techniques de Masuku (Gabon) - Tony Ezome and the PRMAIS project

Start year: 2017

See also: https://www.inria.fr/en/associate-team/fast

The project aims to develop better algorithms for elliptic curve cryptography with prospect of the two challenges ahead: - securing the internet of things - preparing towards quantum computers.

Elliptic curves are currently the fastest public-key cryptosystem (with a key size that can fit on embedded devices) while still through a different mode of operation being (possibly) able to resist quantum based computers.

Activities for this year involved the funding of Luca De Feo to speak at the EMA “Mathématiques pour la Cryptographie Post-quantique et Mathématiques pour le Traitement du Signal”, organised by Djiby Sow and Abdoul Aziz Ciss organised an EMA at the École Polytechnique de Thies (Sénégal) from May 10 to May 23, about “Cryptographie à base d’isogénies”; the visit of Abdoulaye Maiga to the LFANT team where he worked with Damien Robert to find absolute invariants of good reduction modulo 2 for abelian surfaces; and the organisation by Damien Robert of a workshop in Bordeaux with most of the team members from September 04 to September 08. The slides or proceedings are available at https://lfant.math.u-bordeaux.fr/index.php?category=seminar&page=2017.

7.3.2. Inria International Partners

7.3.2.1. Informal International Partners

The team is used to collaborate with Leiden University through the ALGANT program for PhD joint supervision.

Eduardo Friedman (U. of Chile), long term collaborator of K. Belabas and H. Cohen is a regular visitor in Bordeaux (about 1 month every year).

7.4. International Research Visitors

7.4.1. Visits of International Scientists

Researchers visiting the team to give a talk to the team seminar include Damien Stehlé (ENS Lyon), Cécile Pierrot (Centrum Wiskunde and Informatica, Amsterdam), Christophe Petit (Oxford), Benjamin Wesolowski (EPFL), Bernhard Schmidt (Nanyang Technological University, Singapore), Mohamadou Sall (Université Cheikh Anta Diop, Dakar, Sénégal), Emmanuel Fouotsa (The University of Bamenda, Cameroon), Abdoulaye Maiga (Université Cheikh Anta Diop, Dakar, Sénégal), Tony Ezome (Université des Sciences et Techniques de Masuku (USTM), Franceville, Gabon), Abdoul Aziz Ciss (Université Cheikh Anta Diop, Dakar, Sénégal), José Manuel Rodriguez Caballero (Labri), Jean Kieffer (ENS Paris), Christian Klein (Institut de Mathématiques de Bourgogne), Frank Vallentin (Mathematisches Institut, Universität zu Köln).

7.4.2. Visits to International Teams

Jared Asuncion went to the Autumn school: Topics in arithmetic and algebraic geometry last 9 - 13 October 2017 at the University of Mainz in Mainz, Germany.

Jared Asuncion went to see his cosupervisor, Marco String last 6 - 10 November 2017 at the Universiteit Leiden in Leiden, The Netherlands. It is planned to stay in Leiden for a period of six months while working on his PhD.

Jared Asuncion went to the 21st Workshop on Elliptic Curve Cryptography last 13 - 15 November 2017 at the Radboud University in Nijmegen, The Netherlands.
A. Page visited C. Maire in Cornell University (Ithaca, US) from November 27th to December 4th and gave a research talk there on December 1st. He then visited Michael Lipnowski in the Institute for Advanced Studies (Princeton, US) from December 4th to December 14th.

A. Enge visited Bernhard Schmidt in Nanyang Technological University, Singapore for three weeks.

Fredrik Johansson participated in the OSCAR: Antic workshop at TU Kaiserslautern, Germany and gave an invited talk on "Fundamental algorithms in Arb".

Fredrik Johansson participated in the workshop on Elliptic Integrals, Elliptic Functions and Modular Forms in Quantum Field Theory at DESY, Zeuthen, Germany, and gave an invited talk on "Numerics of classical elliptic functions, elliptic integrals and modular forms".

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific Events Organisation

8.1.1.1. General Chair, Scientific Chair

B. Allombert and K. Belabas organized a workshop PARI/GP in Lyon on 09-13 January 2017.

B. Allombert and K. Belabas organized a workshop “Elliptic curves, modular forms and L-functions in the PARI/GP system” in Clermont-Ferrand on 19-23 June 2017.


8.1.2. Journal

8.1.2.1. Member of the Editorial Boards


J.-M. Couveignes is a member of the editorial board (scientific committee) of the Publications mathématiques de Besançon since 2010.

A. Enge is an editor of Designs, Codes and Cryptography since 2004.

8.1.3. Scientific Expertise

J.-M. Couveignes is a member of the scientific council of the labex "Fondation Sciences Mathématiques de Paris", FSMP, Paris.

J.-M. Couveignes is a member of the ‘conseil d’orientation’ of the labex "Institut de Recherche en Mathématiques, Interactions et Applications”, IRMIA, Strasbourg.

K. Belabas is a member of the ‘conseil scientifique’ of the Société Mathématique de France

8.1.4. Research Administration

Since January 2017, A. Enge is “délégué scientifique” of the Inria research centre Bordeaux–Sud-Ouest. As such, he is also a designated member of the “commission d’évaluation” of Inria.

Since January 2015, K. Belabas is vice-head of the Math Institute (IMB). He also leads the computer science support service (“cellule informatique”) of IMB and coordinates the participation of the institute in the regional computation cluster PlaFRIM.

He is an elected member of “commission de la recherche” in the academic senate of Bordeaux University.

He is a member of the “Conseil National des Universités” (25th section, pure mathematics).
J.-P. Cerri is an elected member of the scientific council of the Mathematics Institute of Bordeaux (IMB) and responsible for the bachelor programme in mathematics and informatics.

Since January 2015, J.-M. Couveignes is the head of the Math Institute (IMB). He is head of the Scientific Committee of the Albatros (ALliance Bordeaux universities And Thales Research in AviOnicS) long term cooperation between Inria, Bordeaux-INP, Université de Bordeaux and CNRS.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Master : G. Castagnos, Cryptanalyse, 60h, M2, University of Bordeaux, France;
Master : G. Castagnos, Cryptologie avancée, 30h, M2, University of Bordeaux, France;
Master : G. Castagnos, Courbes elliptiques, 60h, M2, University of Bordeaux, France;
Master : D. Robert, Courbes elliptiques, 60h, M2, University of Bordeaux, France;
Master : K. Belabas, Computer Algebra, 91h, M2, University of Bordeaux, France;
Licence : Jean-Paul Cerri, Arithmétique et Cryptologie, 24h TD, L3, Université de Bordeaux, France
Licence : Jean-Paul Cerri, Algèbre bilinéaire et géométrie, 35h TD, L3, Université de Bordeaux, France
Licence : Jean-Paul Cerri, Structures algébriques 2, 35h TD, L3, Université de Bordeaux, France
Master : Jean-Paul Cerri, Cryptologie, 24h TD, M1, Université de Bordeaux, France
Master : Jean-Paul Cerri, Arithmétique, 60h TD, M1, Université de Bordeaux, France

8.2.2. Supervision

PhD in progress : Ida Tucker, Design of new advanced cryptosystems from homomorphic building blocks, since October 2017, supervised by Guilhem Castagnos and Fabien Laguillaumie.
PhD in progress: Abdoulaye Maiga, Computing canonical lift of genus 2 hyperelliptic curves, University Dakar, supervised by Djiby Sow, Abdoul Aziz Ciss and D. Robert.
PhD in progress: Jared Asuncion, Class fields of complex multiplication fields, since September 2017, supervised by A. Enge and Marco Streng (Universiteit Leiden).
PhD in progress: Chloë Martindale, Isogeny graphs, since 2013, supervised by A. Enge and Marco Streng (Universiteit Leiden).
PhD in progress: Pavel Solomatín Topics on $L$-functions, supervised by B. de Smit and K. Belabas.
PhD in progress: Antonin Riffaut Calcul effectif de points spéciaux, supervised by Y. Bilu and K. Belabas.
Master 2: Margarita Pierrakea, Supersingular isogeny key-exchange, supervised by D. Robert.

8.2.3. Juries

- A. Enge has written a report for the doctoral dissertation by Alexandre Le Meur, Université de Rennes, sur Formules de Thomae généralisées à des courbes galoisiennes résolubles sur la droite projective.
- A. Enge has written a report for the doctoral dissertation by Alexandre Gélin, Université Pierre et Marie Curie, Class Group Computations in Number Fields and Applications to Cryptology. K. Belabas was a member of the defense committee.
- K. Belabas has written a report for the doctoral dissertation of Thomas Camus, Université Grenoble-Alpes, Méthodes algorithmiques pour les réseaux algébriques.
K. Belabas was a member of the defense committee of José Villanueva-Gutierrez, Université de Bordeaux, *Sur quelques questions en théorie d’Iwasawa*.

K. Belabas was a member of the defense committee of Philippe Mounstrou, Université de Bordeaux, *Geometric distance graphs, lattices and polytopes*.

J-M. Couveignes was a member of the defense committee of Carine Jaber (advisor Christian Klein), Université de Dijon, *Approche algorithmique au domaine fondamental de Siegel* the 28 June 2017.

J-M. Couveignes was the president of the defense committee of Matthieu Rambaud (advisor Hugues Randriambololona), Telecom-ParisTech, *Shimura curves and bilinear multiplication algorithms in finite fields* the 2 September 2017.

D. Robert is a member of the jury of Agregations de Mathematiques. He is also the codirector with Alain Couvreur of the option “calcul formel” of the Modelisation part of the oral examination.

### 8.3. Popularization

The book *Guide to Pairing-Based Cryptography* [26] has been published by CHAPMAN and HALL/CRC.

D. Robert wrote with Sorina Ionica the chapter “Pairings” of this book. This book aims to help Engineers understand and implement pairing based cryptography; in the Chapter “Pairings”, D. Robert give a self contained definition and proof of the Weil and Tate pairing; including how to handle divisors with non disjoint support (this is often skipped in scientific papers but is important for practical implementations).

A. Page gave a popularization talk “À la découverte de la cryptologie : la science du secret” during the Fête de la Science event. Two groups of high school students and one group of Inria agents participated in this activity. Following this talk, three high school students decided to work on the RSA cryptosystem for their TPE essay and came back to the IMB to meet A. Page and talk about this topic in greater detail.

### 9. Bibliography

**Major publications by the team in recent years**


Publications of the year

**Articles in International Peer-Reviewed Journal**


**Articles in Non Peer-Reviewed Journal**


**International Conferences with Proceedings**


Scientific Books (or Scientific Book chapters)


Other Publications


[22] A. Page, A. Bartel. Group representations in the homology of 3-manifolds, December 2017, working paper or preprint, https://hal.inria.fr/hal-01671748.

References in notes


Project-Team MAGIQUE-3D

Advanced 3D Numerical Modeling in Geophysics

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

IN PARTNERSHIP WITH:
CNRS
Université de Pau et des Pays de l’Adour

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Earth, Environmental and Energy Sciences
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Project-Team MAGIQUE-3D

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A6.2. - Scientific Computing, Numerical Analysis & Optimization
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.7. - High performance computing

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B5.5. - Materials

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2. Overall Objectives

2.1. General setting

MAGIQUE-3D is a joint project-team between Inria and the Department of Applied Mathematics (LMA) of the University of Pau, in partnership with CNRS. The mission of MAGIQUE-3D is to develop and validate efficient solution methodologies for solving complex three-dimensional geophysical problems, with a particular emphasis on problems arising in seismic imaging, in response to the local industrial and community needs. Indeed, as it is well known, the region of Pau has long-standing tradition in the Geosciences activities. However, in spite of the recent significant advances in algorithmic considerations as well as in computing platforms, the solution of most real-world problems in this field remains intractable. Hence, there is a scientific need of pressing importance to design new numerical methods for solving efficiently and accurately wave propagation problems defined in strongly heterogeneous domains.

MAGIQUE-3D program possesses an exceptional combination that is a prerequisite for accomplishing its mission: the investigator backgrounds, research interests, and technical skills complement to form a research team with a potential for significant impact on the computational infrastructure of geophysical sciences. The research record of MAGIQUE-3D group covers a large spectrum of accomplishments in the field of wave propagation including (a) the design, validation, and performance assessment of a class of DG-methods for solving efficiently high frequency wave problems, (b) the construction, convergence analysis, and performance assessment of various absorbing-type boundary conditions that are key ingredients for solving problems in infinite domains, and (c) the development of asymptotic models that are the primary candidate in the presence of heterogeneities that are small compared to the wave length. MAGIQUE-3D has built strong collaborations and partnerships with various institutions including (a) local industry (TOTAL), (b) national research centers (ONERA and CEA), and (c) international academic partnerships (e.g. Interdisciplinary Research Institute for the Sciences (IRIS) at California State University, Northridge, USA; University of Pays Basque at Bilbao, Spain; University of Novosibirsk, Russia).

3. Research Program

3.1. Introduction

Probing the invisible is a quest that is shared by a wide variety of scientists such as archaeologists, geologists, astrophysicists, physicists, etc... Magique-3D is involved in Geophysical imaging which aims at understanding the internal structure of the Earth from the propagation of waves. Both qualitative and quantitative information are required and two geophysical techniques can be used: seismic reflection and seismic inversion. Seismic
reflection provides a qualitative description of the subsurface from reflected seismic waves by indicating
the position of the reflectors while seismic inversion transforms seismic reflection data into a quantitative
description of the subsurface. Both techniques are inverse problems based upon the numerical solution of
wave equations. Oil and Gas explorations have been pioneering application domains for seismic reflection and
inversion and even if numerical seismic imaging is computationally intensive, oil companies promote the use
of numerical simulations to provide synthetic maps of the subsurface. This is due to the tremendous progresses
of scientific computing which have pushed the limits of existing numerical methods and it is now conceivable
to tackle realistic 3D problems. However, mathematical wave modeling has to be well-adapted to the region
of interest and the numerical schemes which are employed to solve wave equations have to be both accurate
and scalable enough to take full advantage of parallel computing. Today, geophysical imaging tackles more
and more realistic problems and we can contribute to this task by improving the modeling and by deriving
advanced numerical methods for solving wave problems.

Magique-3D proposes to organize its research around three main axes:
1. Mathematical modeling of multi-physics involving wave equations;
2. Supercomputing for Helmholtz problems;
3. Construction of high-order hybrid schemes.

These three research fields will be developed with the main objective of solving inverse problems dedicated to
géophysical imaging.

3.2. Mathematical modeling of multi-physics involving wave equations

Wave propagation modeling is of great interest for many applications like oil and gas exploration, non
destructive testing, medical imaging, etc. It involves equations which can be solved in time or frequency
domain and their numerical approximation is not easy to handle, in particular when dealing with real-world
problems. In both cases, the propagation domain is either infinite or its dimensions are much greater than
the characteristic wavelength of the phenomenon of interest. But since wave problems are hyperbolic, the
physical phenomenon can be accurately described by computing solutions in a bounded domain including the
sources which have generated the waves. Until now, we have mainly worked on imaging techniques based on
acoustic or elastic waves and we have developed advanced finite element software packages which are used
by Total for oil exploration. Nevertheless, research on modeling must go on because there are simulations
which can still not be performed because their computational cost is much too high. This is particularly true
for complex tectonics involving coupled wave equations. We then propose to address the issue of coupling
wave equations problems by working on the mathematical construction of reduced systems. By this way, we
hope to improve simulations of elasto-acoustic and electro-seismic phenomena and then, to perform numerical
imaging of strongly heterogeneous media. Even in the simplest situation where the wavelengths are similar
(elasto-acoustic coupling), the dimension of the discrete coupled problem is huge and it is a genuine issue in
the prospect of solving 3D inverse problems.

The accurate numerical simulation of full wave problems in heterogeneous media is computationally intensive
since it needs numerical schemes based on grids. The size of the cells depends on the propagation velocity
of waves. When coupling wave problems, conversion phenomena may occur and waves with very different
propagation velocity coexist. The size of the cells is then defined from the smallest velocity and in most of the
real-world cases, the computational cost is crippling. Regarding existing computing capabilities, we propose
to derive intermediate models which require less computational burden and provide accurate solutions for a
wide-ranging class of problems including Elasto-acoustics and Electro-seismology.

When it comes to mathematical analysis, we have identified two tasks which could help us simulate realistic
3D multi-physics wave problems and which are in the scope of our savoir-faire. They are construction of
approximate and multiscale models which are different tasks. The construction of approximate problems aims
at deriving systems of equations which discrete formulation involves middle-sized matrices and in general,
they are based on high frequency hypothesis. Multiscale models are based on a rigorous analysis involving a
small parameter which does not depend on the propagation velocity necessarily.
Recently, we have conducted research on the construction of approximate models for offshore imaging. Elastic and acoustic wave equations are coupled and we investigate the idea of eliminating the computations inside water by introducing equivalent interface conditions on the sea bottom. We apply an On-Surface-Radiation-Condition (OSRC) which is obtained from the approximation of the acoustic Dirichlet-to-Neumann (DtN) operator \cite{74}, \cite{53}. To the best of our knowledge, OSRC method has never been used for solving reduced coupling wave problems and preliminary promising results are available at \cite{56}. We would like to investigate this technique further because we could form a battery of problems which can be solved quickly. This would provide a set of solutions which we could use as initial guess for solving inverse problems. But we are concerned with the performance of the OSRC method when wave conversions with different wavelengths occur. Anyway, the approximation of the DtN operator is not obvious when the medium is strongly heterogeneous and multiscale analysis might be more adapted. For instance, according to existing results in Acoustics and Electromagnetism for the modeling of wire antennas \cite{65}, multiscale analysis should turn out to be very efficient when the propagation medium includes well logs, fractures and faults which are very thin structures when compared to the wavelength of seismic waves. Moreover, multiscale analysis should perform well when the medium is strongly oscillating like porous media. It could thus provide an alternative to homogenization techniques which can be applied only when the medium is periodic. We thus propose to develop reduced multi-scale models by performing rigorous mathematical procedure based on regular and singular multiscale analysis. Our approach distinguishes itself from others because it focuses on the numerical representation of small structures by time-dependent problems. This could give rise to the development of new finite element methods which would combine DG approximations with XFEM (Extended Finite Element Method) which has been created for the finite element treatment of thin structures like cracks.

But Earth imaging must be more than using elasto-acoustic wave propagation. Electromagnetic waves can also be used and in collaboration with Prof. D. Pardo (Iker Basque Foundation and University of Bilbao), we conduct researches on passive imaging to probe boreholes. Passive imaging is a recent technique of imaging which uses natural electromagnetic fields as sources. These fields are generated by hydromagnetic waves propagating in the magnetosphere which transform into electromagnetic waves when they reach the ionosphere. This is a mid-frequency imaging technique which applies also to mineral and geothermal exploration, to predict seismic hazard or for groundwater monitoring. We aim at developing software package for resistivity inversion, knowing that current numerical methods are not able to manage 3D inversion. We have obtained results based on a Petrov-Galerkin approximation \cite{50}, but they are limited to 2D cases. We have thus proposed to reduce the 3D problem by using 1D semi-analytic approximation of Maxwell equations \cite{79}. This work has just started in the framework of a PhD thesis and we hope that it will give us the possibility of imaging 3D problems.

Magique-3D would like to expand its know-how by considering electro-seismic problems which are in the scope of coupling electromagnetic waves with seismic waves. Electro-seismic waves are involved in porous media imaging which is a tricky task because it is based on the coupling of waves with very different wavelengths described by Biot equations and Maxwell equations. Biot equations govern waves in saturated porous media and they represent a complex physical phenomenon involving a slow wave which is very difficult to simulate numerically. In \cite{72}, interesting results have been obtained for the simulation of piezoelectric sensors. They are based on a quasi-static approximation of the Maxwell model coupled with Elastodynamics. Now, we are concerned with the capability of using this model for Geophysical Imaging and we believe that the derivation and/or the analysis of suitable modelings is necessary. Collaborations with Geophysicists are thus mandatory in the prospect of using both experimental and numerical approaches. We would like to collaborate with Prof. C. Bordes and Prof. D. Brito (Laboratory of Complex Fluids and their Reservoirs, CNRS and University of Pau) who have efficient experimental devices for the propagation of electromagnetic waves inside saturated porous media \cite{55}. This collaboration should be easy to organize since Magique-3D has a long-term experience in collaborating with geophysicists. We then believe that we will not need a lot of time to get joint results since we can use our advanced software packages Hou10ni and Montjoie and our colleagues have already obtained data. Electro-seismology is a very challenging research domain for us and we would like to enforce our collaborations with IsTerre (Institute of Earth Science, University of Grenoble) and for that topic with Prof. S. Garambois who is an expert in Electro-seismology \cite{81}, \cite{82}, \cite{69}, \cite{70}. A joint research program could gather Geophysicists from the University of Pau and from IsTerre and Magique-3D.
In particular, it would be interesting to compare simulations performed with Hou10ni, Montjoie, with the code developed by Prof. S. Garambois and to use experimental simulations for validation.

3.3. Supercomputing for Helmholtz problems

Probing invisible with harmonic equations is a need for many scientists and it is also a topic offering a wealth of interesting problems for mathematicians. It is well-known that Helmholtz equations discretization is very sensitive to the frequency scale which can be wide-ranging for some applications. For example, depth imaging is searching for deeper layers which may contain hydrocarbons and frequencies must be of a few tens of Hertz with a very low resolution. If it is to detect hidden objects, the depth of the explored region does not exceed a few tens of meters and frequencies close to the kiloHertz are used. High performing numerical methods should thus be stable for a widest as possible frequency range. In particular, these methods should minimize phenomena of numerical pollution that generate errors which increase faster with frequency than with the inverse of space discretization step. As a consequence, there is a need of mesh refinement, in particular at high frequency.

During the period 2010-2014, the team has worked extensively on high order discontinuous Galerkin (DG) methods. Like standard Finite Element Methods, they are elaborated with polynomial basis functions and they are very popular because they are defined locally for each element. It is thus easy to use basis polynomial functions with different degrees and this shows the perfect flexibility of the approximation in case of heterogeneous media including homogeneous parts. Indeed, low degree basis functions can be used in heterogeneous regions where a fine grid is necessary while high degree polynomials can be used for coarse elements covering homogeneous parts. In particular, Magique-3D has developed Hou10ni that solves harmonic wave equations with DG methods and curved elements. We found that both the effects of pollution and dispersion, which are very significant when a conventional finite element method is used, are limited [57]. However, bad conditioning is persisting and reliability of the method is not guaranteed when the coefficients vary considerably. In addition, the number of unknowns of the linear system is too big to hope to solve a realistic 3D problem. So it is important to develop approximation methods that require fewer degrees of freedom. Magique-3D wishes to invest heavily in the development of new approximation methods for harmonic wave equations. It is a difficult subject for which we want to develop different tasks, in collaboration with academic researchers with whom we are already working or have established contacts.

Research directions that we would like to follow are the following.

First, we will continue our long-term collaboration with Prof. Rabia Djellouli. We want to continue to work on hybrid finite element methods that rely on basis functions composed of plane waves and polynomials. These methods have demonstrated good resistance to the phenomenon of numerical pollution [51], [52], but their capability of solving industrial problems has not been illustrated. This is certainly due to the absence of guideline for choosing the plane waves. We are thus currently working on the implementation of a methodology that makes the choice of plane waves automatic for a given simulation (fixed propagation domain, data source, etc.). This is up-front investigation and there is certainly a lot of remaining work before being applied to geophysical imaging. But it gives the team the opportunity to test new ideas while remaining in contact with potential users of the methods.

Then we want to work with Prof. A. Bendali on developing methods of local integral equations which allow calculation of numerical fluxes on the edges of elements. One could then use these fluxes in a DG method for reconstructing the solution throughout the volume of calculation. This research is motivated by recent results which illustrate the difficulties of the existing methods which are not always able to approximate the propagating modes (plane waves) and the evanescent modes (polynomials) that may coexist, especially when one considers realistic applications. Integral equations are direct tools for computing fluxes and they are known for providing very good accuracy. They thus should help to improve the quality of approximation of DG methods which are fully flux-dependent. In addition, local integral equations would limit calculations at the interfaces, which would have the effect of limiting the number of unknowns generally high, especially for DG methods. Again, it is a matter of long-term research which success requires a significant amount of mathematical analysis, and also the development of non-trivial code.
To limit the effects of pollution and dispersion is not the only challenge that the team wants to tackle. Our experience alongside Total has made us aware of the difficulties in constructing meshes that are essential to achieve our simulations. There are several teams at Inria working on mesh generation and we are in contact with them, especially with Gamma3 (Paris-Rocquencourt Research Center). These teams develop meshes increasingly sophisticated to take account of the constraints imposed by realistic industrial benchmarks. But in our opinion, issues which are caused by the construction of meshes are not the only downside. Indeed, we have in mind to solve inverse problems and in this case it is necessary to mesh the domain at each iteration of Newton-type solver. It is therefore interesting to work on methods that either do not use mesh or rely on meshes which are very easy to construct. Regarding meshless methods, we have begun a collaboration with Prof. Djellouli which allowed us to propose a new approach called Mesh-based Frontier Free Formulation (MF3). The principle of this method is the use of fundamental solutions of Helmholtz equations as basis functions. One can then reduce the volumic variational formulation to a surfacic variational formulation which is close to an integral equation, but which does not require the calculation of singularities. The results are very promising and we hope to continue our study in the context of the application to geophysical imaging. An important step to validate this method will be particularly its extension to 3D because the results we have achieved so far are for 2D problems.

Keeping in mind the idea of limiting the difficulties of mesh, we want to study the method of virtual elements. This method attracts us because it relies on meshes that can be made of arbitrarily-shaped polygon and meshes should thus be fairly straightforward. Existing works on the subject have been mainly developed by the University of Pavia, in collaboration with Los Alamos National Laboratory [54], [61], [60], [58], [62]. None of them mentions the feasibility of the method for industrial applications and to our knowledge, there are no results on the method of virtual elements applied to the wave equations. First, we aim at applying the method described in [59] to the scalar Helmholtz equation and explore opportunities to use discontinuous elements within this framework. Then hp-adaptivity could be kept, which is particularly interesting for wave propagation in heterogeneous media.

DG methods are known to require a lot of unknowns that can exceed the limits accepted by the most advanced computers. This is particularly true for harmonic wave equations that require a large number of discretization points, even in the case of a conventional finite element method. We therefore wish to pursue a research activity that we have just started in collaboration with the project-team Nachos (Sophia-Antipolis Méditerranée Research Center). In order to reduce the number of degrees of freedom, we are interested in "hybrid mixed" Discontinuous Galerkin methods that provides a two-step procedure for solving the Helmholtz equations [73], [77], [76]. First, Lagrange multipliers are introduced to represent the flux of the numerical solution through the interface (edge or face) between two elements. The Lagrange multipliers are solution to a linear system which is constructed locally element by element. The number of degrees of freedom is then strongly reduced since for a standard DG method, there is a need of considering unknowns including volumetric values inside the element. And obviously, the gain is even more important when the order of the element is high. Next, the solution is reconstructed from the values of the multipliers and the cost of this step is negligible since it only requires inverting small-sized matrices. We have obtained promising results in the framework of the PhD thesis of Marie Bonnasse-Gahot and we want to apply it to the simulation of complex phenomena such as the 3D viscoelastic wave propagation.

Obviously, the success of all these works depends on our ability to consider realistic applications such as wave propagation in the Earth. And in these cases, it is quite possible that even if we manage to develop accurate less expensive numerical methods, the solution of inverse problems will still be computationally intensive. It is thus absolutely necessary that we conduct our research by taking advantage of the latest advances in high-performance computing. We have already initiated discussions with the project team HIEPACS (Bordeaux Sud-Ouest research Center) to test the performance of the latest features of Mumps http://mumps.enseeiht.fr/, such as Low Rank Approximation or adaptation to hybrid CPU / GPU architectures and to Intel Xeon Phi, on realistic test cases. We are also in contact with the team Algorithm at Cerfacs (Toulouse) for the development of local integral equations solvers. These collaborations are essential for us and we believe that they will be decisive for the simulation of three-dimensional elasto-dynamic problems. However, our scientific contribution will be limited in this area because we are not experts in HPC.
3.4. Hybrid time discretizations of high-order

Most of the meshes we consider are composed of cells greatly varying in size. This can be due to the physical characteristics (propagation speed, topography, ...) which may require to refine the mesh locally, very unstructured meshes can also be the result of dysfunction of the mesher. For practical reasons which are essentially guided by the aim of reducing the number of matrix inversions, explicit schemes are generally privileged. However, they work under a stability condition, the so-called Courant Friedrichs Lewy (CFL) condition which forces the time step being proportional to the size of the smallest cell. Then, it is necessary to perform a huge number of iterations in time and in most of the cases because of a very few number of small cells. This implies to apply a very small time step on grids mainly composed of coarse cells and thus, there is a risk of creating numerical dispersion that should not exist. However, this drawback can be avoided by using low degree polynomial basis in space in the small meshes and high degree polynomials in the coarse meshes. By this way, it is possible to relax the CFL condition and in the same time, the dispersion effects are limited. Unfortunately, the cell-size variations are so important that this strategy is not sufficient. One solution could be to apply implicit and unconditionally stable schemes, which would obviously free us from the CFL constraint. Unfortunately, these schemes require inverting a linear system at each iteration and thus needs huge computational burden that can be prohibitive in 3D. Moreover, numerical dispersion may be increased. Then, as second solution is the use of local time stepping strategies for matching the time step to the different sizes of the mesh. There are several attempts [66], [63], [80], [75], [68] and Magique 3D has proposed a new time stepping method which allows us to adapt both the time step and the order of time approximation to the size of the cells. Nevertheless, despite a very good performance assessment in academic configurations, we have observed to our detriment that its implementation inside industrial codes is not obvious and in practice, improvements of the computational costs are disappointing, especially in a HPC framework. Indeed, the local time stepping algorithm may strongly affect the scalability of the code. Moreover, the complexity of the algorithm is increased when dealing with lossy media [71].

Recently, Dolean et al [67] have considered a novel approach consisting in applying hybrid schemes combining second order implicit schemes in the thin cells and second order explicit discretization in the coarse mesh. Their numerical results indicate that this method could be a good alternative but the numerical dispersion is still present. It would then be interesting to implement this idea with high-order time schemes to reduce the numerical dispersion. The recent arrival in the team of J. Chabassier should help us to address this problem since she has the expertise in constructing high-order implicit time scheme based on energy preserving Newmark schemes [64]. We propose that our work be organized around the two following tasks. The first one is the extension of these schemes to the case of lossy media because applying existing schemes when there is attenuation is not straightforward. This is a key issue because there is artificial attenuation when absorbing boundary conditions are introduced and if not, there are cases with natural attenuation like in viscoelastic media. The second one is the coupling of high-order implicit schemes with high-order explicit schemes. These two tasks can be first completed independently, but the ultimate goal is obviously to couple the schemes for lossy media. We will consider two strategies for the coupling. The first one will be based on the method proposed by Dolean et al, the second one will consist in using Lagrange multiplier on the interface between the coarse and fine grids and write a novel coupling condition that ensures the high order consistency of the global scheme. Besides these theoretical aspects, we will have to implement the method in industrial codes and our discretization methodology is very suitable for parallel computing since it involves Lagrange multipliers. We propose to organize this task as follows. There is first the crucial issue of a systematic distribution of the cells in the coarse/explicit and in the fine/implicit part. Based on our experience on local time stepping, we claim that it is necessary to define a criterion which discriminates thin cells from coarse ones. Indeed, we intend to develop codes which will be used by practitioners, in particular engineers working in the production department of Total. It implies that the code will be used by people who are not necessarily experts in scientific computing. Considering real-world problems means that the mesh will most probably be composed of a more or less high number of subsets arbitrarily distributed and containing thin or coarse cells. Moreover, in the prospect of solving inverse problems, it is difficult to assess which cells are thin or not in a mesh which varies at each iteration.
Another important issue is the load balancing that we cannot avoid with parallel computing. In particular, we will have to choose one of these two alternatives: dedicate one part of processors to the implicit computations and the other one to explicit calculus or distribute the resolution with both schemes on all processors. A collaboration with experts in HPC is then mandatory since we are not expert in parallel computing. We will thus continue to collaborate with the team-projects HiPacS and Runtime with whom we have a long-term experience of collaborations.

In the future, we aim at enlarging the application range of implicit schemes. The idea will be to use the degrees of freedom offered by the implicit discretization in order to tackle specific difficulties that may appear in some systems. For instance, in systems involving several waves (as P and S waves in porous elastic media, or coupled wave problems as previously mentioned) the implicit parameter could be adapted to each wave and optimized in order to reduce the computational cost. More generally, we aim at reducing numeric bottlenecks by adapting the implicit discretization to specific cases.

4. Application Domains

4.1. Seismic Imaging

The main objective of modern seismic processing is to find the best representation of the subsurface that can fit the data recorded during the seismic acquisition survey. In this context, the seismic wave equation is the most appropriate mathematical model. Numerous research programs and related publications have been devoted to this equation. An acoustic representation is suitable if the waves propagate in a fluid. But the subsurface does not contain fluids only and the acoustic representation is not sufficient in the general case. Indeed the acoustic wave equation does not take some waves into account, for instance shear waves, turning waves or the multiples that are generated after several reflections at the interfaces between the different layers of the geological model. It is then necessary to consider a mathematical model that is more complex and resolution techniques that can model such waves. The elastic or viscoelastic wave equations are then reference models, but they are much more difficult to solve, in particular in the 3D case. Hence, we need to develop new high-performance approximation methods.

Reflection seismics is an indirect measurement technique that consists in recording echoes produced by the propagation of a seismic wave in a geological model. This wave is created artificially during seismic acquisition surveys. These echoes (i.e., reflections) are generated by the heterogeneities of the model. For instance, if the seismic wave propagates from a clay layer to sand, one will observe a sharp reflected signal in the seismic data recorded in the field. One then talks about reflection seismics if the wave is reflected at the interface between the two media, or talks about seismic refraction if the wave is transmitted along the interface. The arrival time of the echo enables one to locate the position of this transition, and the amplitude of the echo gives information on some physical parameters of the two geological media that are in contact. The first petroleum exploration surveys were performed at the beginning of the 1920’s and for instance, the Orchard Salt Dome in Texas (USA) was discovered in 1924 by the seismic-reflection method.

4.2. Imaging complex media with ultrasonic waves

The acoustic behavior of heterogeneous or composite materials attracts considerable excitement. Indeed, their acoustic response may be extremely different from the single constituents responses. In particular, dispersions of resonators in a matrix are the object of large research efforts, both experimentally and theoretically. However it is still a challenge to dispose of numerical tools with sufficient abilities to deal with the simulation and imaging of such materials behavior. Indeed, not only acoustic simulations are very time-consuming, but they have to be performed on realistic enough solution domains, i.e. domains which capture well enough the structural features of the considered materials.

This collaboration with I2M, University of Bordeaux aims at addressing this type of challenges by developing numerical and experimental tools in order to understand the propagation of ultrasonic waves in complex media, image these media, and in the future, help design composite materials for industrial purposes.
4.3. Helioseismology

This collaboration with the Max Planck Institute for Solar System, Göttingen, Germany, which started in 2014, aims at designing efficient numerical methods for the wave propagation problems that arise in helioseismology in the context of inverse problems. The final goal is to retrieve information about the structure of the Sun i.e. inner properties such as density or pressure via the inversion of a wave propagation problem. Acoustic waves propagate inside the Sun which, in a first approximation and regarding the time scales of physical phenomena, can be considered as a moving fluid medium with constant velocity of motion. Some other simplifications lead to computational saving, such as supposing a radial or axisymmetric geometry of the Sun. Aeroacoustic equations must be adapted and efficiently solved in this context, this has been done in the finite elements code Montjoie. In other situations, a full 3D simulation is required and demands large computational resources. Ultimately, we aim at modeling the coupling with gravity potential and electromagnetic waves (MHD equations) in order to be able to better understand Sun spots.

5. New Software and Platforms

5.1. Elasticus

**KEYWORDS**: Discontinuous Galerkin - Acoustic equation - Elastodynamic equations - Elastoacoustic - 2D - 3D - Time Domain

**SCIENTIFIC DESCRIPTION**: Elasticus simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

**FUNCTIONAL DESCRIPTION**: Elasticus is a sequential library, independent of Total plateform and developped in Fortran, to simulate wave propagation in geophysical environment, based on a DG method. It is meant to help PhD students and post-doctoral fellows to easily implement their algorithms in the library. Thus, readability of the code is privileged to optimization of its performances. Developed features should be easily transferred in the computing platform of Total. Elasticus manages arbitrary orders for the spatial discretization with DG method.

**NEWS OF THE YEAR**: In 2017, we implemented the coupling between triangles and quadrangles, and we started the implementation of coupling between Discontinuous Galerkin methods and Spectral Element methods

- Participants: Julien Diaz, Lionel Boillot and Simon Ettouati
- Partner: TOTAL
- Contact: Julien Diaz

5.2. Hou10ni

**KEYWORDS**: 2D - 3D - Elastodynamic equations - Acoustic equation - Elastoacoustic - Frequency Domain - Time Domain - Discontinuous Galerkin

**SCIENTIFIC DESCRIPTION**: Hou10ni simulates acoustic and elastic wave propagation in time domain and in harmonic domain, in 2D and in 3D. It is also able to model elasto acoustic coupling. It is based on the second order formulation of the wave equation and the space discretization is achieved using Interior Penalty Discontinuous Galerkin Method. Recently, the harmonic domain solver has been extended to handle Hybridizable Discontinuous Galerkin Methods.

**FUNCTIONAL DESCRIPTION**: This software simulates the propagation of waves in heterogeneous 2D and 3D media in time-domain and in frequency domain. It is based on an Interior Penalty Discontinuous Galerkin Method (IPDGM) and allows for the use of meshes composed of cells of various order (p-adaptivity in space).
NEWS OF THE YEAR: In 2017, we have completed the implementation of hybridizable DG for 3D anisotropic elastic, and we have coupled Hou10ni with Maphys (developed by Inria team project Hiepacs). We have begun scalability tests and performance comparison of Hou10ni/Mumps vs Hou10ni/Maphys, in the framework of the european project HPC4E.

- Participants: Conrad Hillairet, Elodie Estecahandy, Julien Diaz, Lionel Boillot and Marie Bonnasse Gahot
- Contact: Julien Diaz
- Hybridizable Discontinuous Galerkin method for the simulation of the propagation of the elastic wave equations in the frequency domain - Discontinuous Galerkin methods for the simulation of the propagation of the elastic wave equations in the frequency domain - High order discontinuous Galerkin methods for time-harmonic elastodynamics - Hybridizable discontinuous Galerkin method for the two-dimensional frequency-domain elastic wave equations - Efficient DG-like formulation equipped with curved boundary edges for solving elasto-acoustic scattering problems - Numerical schemes for the simulation of seismic wave propagation in frequency domain - Performance analysis of DG and HDG methods for the simulation of seismic wave propagation in harmonic domain - Hybridizable Discontinuous Galerkin method for solving Helmholtz elastic wave equations - Discontinuous Galerkin methods for solving Helmholtz elastic wave equations for seismic imaging - Performance comparison of HDG and classical DG method for the simulation of seismic wave propagation in harmonic domain - Contributions to the mathematical modeling and to the parallel algorithmic for the optimization of an elastic wave propagator in anisotropic media - Contribution to the mathematical analysis and to the numerical solution of an inverse elasto-acoustic scattering problem
- URL: https://team.inria.fr/magique3d/software/hou10ni/

5.3. MONTJOIE

KEYWORDS: High order finite elements - Edge elements - Aeroacoustics - High order time schemes
**Scientific Description:** Montjoie is designed for the efficient solution of time-domain and time-harmonic linear partial differential equations using high-order finite element methods. This code is mainly written for quadrilateral/hexahedral finite elements, partial implementations of triangular/tetrahedral elements are provided. The equations solved by this code, come from the "wave propagation" problems, particularly acoustic, electromagnetic, aeroacoustic, elastodynamic problems.

**Functional Description:** Montjoie is a code that provides a C++ framework for solving partial differential equations on unstructured meshes with finite element-like methods (continuous finite element, discontinuous Galerkin formulation, edge elements and facet elements). The handling of mixed elements (tetrahedra, prisms, pyramids and hexahedra) has been implemented for these different types of finite elements methods. Several applications are currently available: wave equation, elastodynamics, aeroacoustics, Maxwell’s equations.

- **Participants:** Gary Cohen, Juliette Chabassier, Marc Duruflé and Morgane Bergot
- **Contact:** Marc Duruflé
- **URL:** http://montjoie.gforge.inria.fr/

### 5.4. tmodeling-DG

**Time-domain Wave-equation Modeling App**

**Keywords:** 2D - 3D - Elastoacoustic - Elastodynamic equations - Discontinuous Galerkin - Time Domain

**Scientific Description:** tmodeling-DG simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

**Functional Description:** tmodelling-DG is the follow up to DIVA-DG that we develop in collaboration with our partner Total. Its purpose is more general than DIVA-DG and should contains various DG schemes, basis functions and time schemes. It models wave propagation in acoustic media, elastic (isotropic and TTI) media and elasto-acoustic media, in two and three dimensions.

**News of the Year:** In 2017, we have completed the implementation of Lagrange and Jacobi polynomials and we have released the 3D elastodynamic version and the 3D elasto-acoustic coupling.

- **Participants:** Julien Diaz, Lionel Boillot and Simon Ettouati
- **Partner:** TOTAL
- **Contact:** Julien Diaz

### 5.5. fmodeling

**Frequency-domain Wave-equation Modeling App (fModeling)**

**Keywords:** Discontinuous Galerkin - Frequency Domain - 2D - 3D - Elastodynamic equations - Acoustic equation

**Scientific Description:** FModelling simulates acoustic and elastic wave propagation in frequency domain, in 2D and in 3D, using Discontinuous Galerkin Methods and Hybridizable Discontinuous Galerkin Methods. The space discretization is based on Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with two linear solvers (Mumps and Maphys).

**Functional Description:** fmodeling is developed in partnership with Total in the context of the Depth Imaging Partnership (DIP). It is the equivalent of Tmodeling for frequency domain. The software deals with wave equation in the frequency domain and solves the forward problem using Discontinuous Galerkin methods or Hybridizable Discontinuous Galerkin Methods. In particular, acoustic and elastic (isotropic and TTI) media are considered in two and three dimensions. It is planned to implement and to test various kind of basis function and to couple the code with various linear solvers (such as Mumps or Maphys). The software is coupled to the Inversion solver of Total to conduct Sesimic Imaging using iterative minimization with the Full Waveform Inversion method.
NEWS OF THE YEAR: In 2017, we completed the implementation of Hybridizable Discontinuous Galerkin Methods and we started the validation of the code in an industrial context. We have also coupled the code with the Full Waveform Inversion solver of Total.

- Partner: TOTAL
- Contact: Julien Diaz

6. New Results

6.1. Seismic Imaging and Inverse Problems


**Participants:** Hélène Barucq, Elodie Estecahandy.

The characterization of the Fréchet derivative of the elasto-acoustic scattered field with respect to Lipschitz continuous polygonal domains is established. The considered class of domains is of practical interest since two-dimensional scatterers are always transformed into polygonal-shaped domains when employing finite element methods for solving direct and inverse scattering problems. The obtained result indicates that the Fréchet derivative with respect to the scatterer of the scattered field is the solution of the same elasto-acoustic scattering problem but with additional right-hand side terms in the transmission conditions across the fluid-structure interface. This characterization has the potential to advance the state-of-the-art of the solution of inverse obstacle problems. This work has been done in collaboration with Prof. Rabia Djellouli (California State University at Northridge) and has been accepted for publication in Siam Journal of Applied Mathematics [16].

6.1.2. Shape-reconstruction and parameter identification of an elastic object immersed in a fluid

**Participants:** Izar Azpiroz Iragorri, Hélène Barucq, Julien Diaz, Kevin Lagnoux.

We have developed a procedure to reconstruct the shape and material parameters of an elastic obstacle immersed in a fluid medium from some external measurements given by the so called far-field pattern. It is a nonlinear and ill-posed problem which is solved by applying a Newton-like iterative method involving the Fréchet derivatives of the scattered field. These derivatives express the sensitivity of the scattered field with respect to the parameters of interest. They are defined as the solution of boundary value problems which differ from the direct one only at the right-hand sides level. We have been able to establish the well-posedness of each problem in the case of a regular obstacle and it would be interesting in the near future to extend those results to the case of scatterers with polygonal boundaries. It requires to work with less regular Sobolev spaces for which the definition of traces is not obvious. We have also provided an analytical representation of the Fréchet derivatives in the case of a circle. This provide a way of validating the numerical experiments and it would be interesting to extend it to anisotropic media as well. It requires to establish analytic representations of the scattered field in anisotropic media which is more difficult because it involves more parameters.
We have studied the response of the data to the different parameters. It turns out that the sensitivity of the far field pattern is very different regarding the shape or the material parameters. We have delivered a sensitivity analysis which has been essential for understanding that the reconstruction of the material parameters is conditioned by the recovering of the shape parameters. This makes the full reconstruction very difficult and sometimes unstable. In particular, in the case of a disk-shaped obstacle, when addressing the role of the frequency in the reconstruction, we have been faced to the issue of the existence of Jones modes which had been already observed by Elodie Estecahandy in her PhD thesis. Next, we have introduced a series of numerical experiments that have been performed by applying two algorithms which propose two strategies of full reconstruction regarding the material parameters are retrieved simultaneously with the shape or not. It turns out that both work similarly delivering the same level of accuracy but the simultaneous reconstruction requires less iterations. We have thus opted for retrieving all the parameters simultaneously. Since realistic configurations include noisy data, we have performed some simulations for the reconstruction of the shape along with the Lamé coefficients for different noise levels. Other interesting experiments have been carried out using a multistage procedure where the parameters of interest are the density of the solid interior, the shape of the obstacle and its position. We have considered the case of Limited Aperture Data in back-scattering configurations, using multiple incident plane waves, mimicking a physical disposal of non-destructive testing. This is an encouraging ongoing work which deserves to be completed by considering a wide range of examples including more general geometries of the scatterer. It should also be extended by dealing with limited aperture data using only one incident wave (which will probably require multiple frequency data).

These results have been obtained in collaboration with Rabia Djellouli (California State University at Northridge, USA) and were presented to the Waves 2017 conference.

6.1.3. Shape-reconstruction and parameter identification of an anisotropic elastic object immersed in a fluid

**Participants:** Izar Azpiroz Iragorri, Hélène Barucq, Julien Diaz.

We extended the solution methodology for reconstructing the shape and material parameters of an elastic obstacle (see 6.1.2) to the case of anisotropic media. This is a very challenging case which still deserves further works. We have obtained some results but since the impact of some of the anisotropic parameters on the FFP is even weaker than the Lamé coefficients, the reconstruction of these parameters together with the shape parameters requires several frequencies and carefully adapted regularization parameters. It is in particular difficult to retrieve the Thomsen parameters $\epsilon$ and $\delta$ because their reconstruction requires to have an accurate adjustment on the rest of material and shape parameters. The recovery process is thus computationally intensive and some efforts should be done in the near future to decrease the computational costs. We were able to recover all the anisotropic parameters when the shape were assumed to be known. However, when trying to recover both shape and material parameters, we could only recover the shape and some of the physical parameters (namely the three most important ones: the density and the two velocities $V_p$ and $V_s$). We should now find a way to determine all the Thomsen parameters together with the shape. Then, we will have to deal with more complex media such as TTI media (this will add the angle of anisotropy as additional parameter). The last step will be to consider general anisotropy, which could be done by recovering each element of the elastic stiffness tensor. This is simple to implement, since the derivative of the stiffness tensor with respect to one of its component is easily computable (it is a tensor composed of zeroes and ones). However, the stability of the reconstruction is not guaranteed, since we will strongly increase the number of components to be retrieved.

These results have been obtained in collaboration with Rabia Djellouli (California State University at Northridge, USA).

6.1.4. Mathematical analysis and solution methodology for a class of inverse spectral problems arising in the design of optical waveguides

**Participant:** Hélène Barucq.
We analyze mathematically the problem of determining refractive index profiles from some desired/measured guided waves propagating in optical fibers. We establish the uniqueness of the solution of this inverse spectral problem assuming that only one guided mode is known. Then, we propose an iterative computational procedure for solving numerically the considered inverse spectral problem. Numerical results are presented to illustrate the potential of the proposed regularized Newton algorithm to efficiently and accurately retrieve the refractive index profiles even when the guided mode measurements are highly noisy.

This work has been submitted for publication in a peer-reviewed journal. It has been done in collaboration with Rabia Djellouli (California State University at Northridge, USA) and Chokri Bekkey (University of Monastir, Tunisia)

6.1.5. Time-harmonic seismic inverse problem with Cauchy data

**Participants:** Florian Faucher.

This work is a collaboration with Giovanni Alessandrini (Università di Trieste), Maarten V. de Hoop (Rice University), Romina Gaburro (University of Limerick) and Eva Sincich (Università di Trieste).

We study the performance of Full Waveform Inversion (FWI) from time-harmonic Cauchy data via conditional well-posedness driven iterative regularization. The Cauchy data can be obtained with dual sensors measuring the pressure and the normal velocity. We define a novel misfit functional which, adapted to the Cauchy data, allows the independent location of experimental and computational sources. The conditional well-posedness is obtained for a hierarchy of subspaces in which the inverse problem with partial data is Lipschitz stable. Here, these subspaces yield piecewise linear representations of the wave speed on given domain partitions. Domain partitions can be adaptively obtained through segmentation of the gradient. The domain partitions can be taken as a coarsening of an unstructured tetrahedral mesh associated with a finite element discretization of the Helmholtz equation. We illustrate the effectiveness of the iterative regularization through computational experiments with data in dimension three. In comparison with earlier work, the Cauchy data do not suffer from eigenfrequencies in the configurations.

The resulting paper is [47] and is also connected to the following conference presentations, [36], [27].

6.1.6. Quantitative Convergence of Full Waveform Inversion in the Frequency Domain

**Participants:** Hélène Barucq, Florian Faucher.

This work is a collaboration with Guy Chavent (Inria Rocquencourt).

We study the convergence of the inverse problem associated with the frequency domain wave equations for the recovery of subsurface parameters. The numerical method selected for the resolution is the Full Waveform Inversion (FWI), which designs an iterative minimization algorithm. We study the convergence of the scheme in the context of least squares minimization. We establish numerical estimates based on the Fréchet derivatives for the radius of curvature and the deflection. We quantify the (complex) frequency progression to select to foster the convergence, and illustrate the effect of the subsurface geometry. From the curvature estimates, we also provide an insight of the robustness with noise depending on the situation. We supplement the numerical analysis with numerical experiments to demonstrate the results.

The results have been presented in the following conference, [36], [27], [26], [25].

6.1.7. Contributions to seismic full waveform inversion for time harmonic wave equations: stability estimates, convergence analysis, numerical experiments involving large scale optimization algorithms

**Participants:** Hélène Barucq, Florian Faucher.

In this project, we investigate the recovery of subsurface Earth parameters. We consider the seismic imaging as a large scale iterative minimization problem, and deploy the Full Waveform Inversion (FWI) method. The reconstruction is based on the wave equations because the characteristics of the measurements indicate the nature of the medium in which the waves propagate. First, the natural heterogeneity and anisotropy of the Earth require numerical methods that are adapted and efficient to solve the wave propagation problem. In this study, we have decided to work with the harmonic formulation, i.e., in the frequency domain.
The inverse problem is then established in order to frame the seismic imaging. It is a nonlinear and ill-posed inverse problem by nature, due to the limited available data, and the complexity of the subsurface characterization. However, we obtain a conditional Lipschitz-type stability in the case of piecewise constant model representation. We derive the lower and upper bound for the underlying stability constant, which allows us to quantify the stability with frequency and scale. It is of great use for the underlying optimization algorithm involved to solve the seismic problem. We review the foundations of iterative optimization techniques and provide the different methods that we have used in this project. The Newton method, due to the numerical cost of inverting the Hessian, may not always be accessible. We propose some comparisons to identify the benefits of using the Hessian, in order to study what would be an appropriate procedure regarding the accuracy and time. We study the convergence of the iterative minimization method, depending on different aspects such as the geometry of the subsurface, the frequency, and the parametrization. In particular, we quantify the frequency progression, from the point of view of optimization, by showing how the size of the basin of attraction evolves with frequency.

Following the convergence and stability analysis of the problem, the iterative minimization algorithm is conducted via a multi-level scheme where frequency and scale progress simultaneously. We perform a collection of experiments, including acoustic and elastic media, in two and three dimensions. The perspectives of attenuation and anisotropic reconstructions are also introduced.

6.1.8. Quantitative localization of small obstacles with single-layer potential fast solvers

Participants: Hélène Barucq, Florian Faucher, Ha Pham.

In this work, we numerically study the inverse problem of locating small circular obstacles in a homogeneous medium using noisy backscattered data collected at several frequencies. The main novelty of our work is the implementation of a single-layer potential based fast solver (called FSSL) in a Full-Waveform inversion procedure, to give high quality reconstruction with low-time cost. The efficiency of FSSL was studied in our previous works. We show reconstruction results with up to 12 obstacles in structured or random configurations with several initial guesses, all allowed to be far and different in nature from the target. This last assumption is not expected in results using nonlinear optimization schemes in general. For results with 6 obstacles, we also investigate several optimization methods, comparing between nonlinear gradient descent and quasi-Newton, as well as their convergence with different line search algorithms.

The resulting research report is [45].

6.2. Mathematical modeling of multi-physics involving wave equations

6.2.1. Atmospheric Radiation Boundary Conditions for the Helmholtz Equation

Participants: Hélène Barucq, Juliette Chabassier, Marc Duruflé.

An article is to be published in M2AN, see [14]. This work offers some contributions to the numerical study of acoustic waves propagating in the Sun and its atmosphere. The main goal is to provide boundary conditions for outgoing waves in the solar atmosphere where it is assumed that the sound speed is constant and the density decays exponentially with radius. Outgoing waves are governed by a Dirichlet-to-Neumann map which is obtained from the factorization of the Helmholtz equation expressed in spherical coordinates. For the purpose of extending the outgoing wave equation to axisymmetric or 3D cases, different approximations are implemented by using the frequency and/or the angle of incidence as parameters of interest. This results in boundary conditions called Atmospheric Radiation Boundary Conditions (ARBC) which are tested in ideal and realistic configurations. These ARBCs deliver accurate results and reduce the computational burden by a factor of two in helioseismology applications. This work has been done in collaboration with Laurent Gizon and Michael Leguèbe (Max-Planck-Institut für Sonnensystemforschung, Gottingen, Germany).
6.2.2. Atmospheric radiation boundary conditions for high frequency waves in time-distance helioseismology

Participants: Hélène Barucq, Juliette Chabassier, Marc Duruflé.

An article has been published in Astronomy and Astrophysics [22]. The temporal covariance between seismic waves measured at two locations on the solar surface is the fundamental observable in time-distance helioseismology. Above the acoustic cutoff frequency (5.3 mHz), waves are not trapped in the solar interior and the covariance function can be used to probe the upper atmosphere. We wish to implement appropriate radiative boundary conditions for computing the propagation of high-frequency waves in the solar atmosphere. We consider the radiative boundary conditions recently developed by Barucq et al. (2017) for atmospheres in which sound-speed is constant and density decreases exponentially with radius. We compute the cross-covariance function using a finite element method in spherical geometry and in the frequency domain. The ratio between first-and second-skip amplitudes in the time-distance diagram is used as a diagnostic to compare boundary conditions and to compare with observations. We find that a boundary condition applied 500 km above the photosphere and derived under the approximation of small angles of incidence accurately reproduces the ‘infinite atmosphere’ solution for high-frequency waves. When the radiative boundary condition is applied 2 Mm above the photosphere, we find that the choice of atmospheric model affects the time-distance diagram. In particular, the time-distance diagram exhibits double-ridge structure when using a VAL atmospheric model. This is a collaboration with Damien Fournier, Laurent Gizon, Chris Hanson and Michael Leguèbe (Max-Planck-Institut für Sonnensystemforschung, Gottingen, Germany).

6.2.3. Computational helioseismology in the frequency domain: acoustic waves in axisymmetric solar models with flows

Participants: Hélène Barucq, Juliette Chabassier, Marc Duruflé.

An article has been published in Astronomy and Astrophysics [23]. Context. Local helioseismology has so far relied on semi-analytical methods to compute the spatial sensitivity of wave travel times to perturbations in the solar interior. These methods are cumbersome and lack flexibility. Aims. Here we propose a convenient framework for numerically solving the forward problem of time-distance helioseismology in the frequency domain. The fundamental quantity to be computed is the cross-covariance of the seismic wavefield. Methods. We choose sources of wave excitation that enable us to relate the cross-covariance of the oscillations to the Green’s function in a straightforward manner. We illustrate the method by considering the 3D acoustic wave equation in an axisymmetric reference solar model, ignoring the effects of gravity on the waves. The symmetry of the background model around the rotation axis implies that the Green’s function can be written as a sum of longitudinal Fourier modes, leading to a set of independent 2D problems. We use a high-order finite-element method to solve the 2D wave equation in frequency space. The computation is embarrassingly parallel, with each frequency and each azimuthal order solved independently on a computer cluster. Results. We compute travel-time sensitivity kernels in spherical geometry for flows, sound speed, and density perturbations under the first Born approximation. Convergence tests show that travel times can be computed with a numerical precision better than one millisecond, as required by the most precise travel-time measurements. Conclusions. The method presented here is computationally efficient and will be used to interpret travel-time measurements in order to infer, e.g., the large-scale meridional flow in the solar convection zone. It allows the implementation of (full-waveform) iterative inversions, whereby the axisymmetric background model is updated at each iteration. This work is a collaboration with Aaron Birch, Damien Fournier, Laurent Gizon, Chris Hanson, Michael Leguèbe and Emanuele Papini (Max-Planck-Institut für Sonnensystemforschung, Gottingen, Germany) and with Thorsten Hohage (Göttingen University, Germany).

6.2.4. The virtual workshop: towards versatile optimal design of musical wind instruments for the makers

Participants: Juliette Chabassier, Robin Tournemenne.

Our project aims at proposing optimization solutions for wind instrument making. Our approach is based on a strong interaction with makers and players, aiming at defining interesting criteria to optimize from their point
of view. After having quantified those criteria under the form of a cost function and a design parameters space, we wish to implement state-of-the-art numerical methods (finite elements, full waveform inversion, neuronal networks, diverse optimization techniques...) that are versatile (in terms of models, formulations, couplings...) in order to solve the optimization problem. More precisely, we wish to take advantage of the fact that sound waves in musical instruments satisfy the laws of acoustics in pipes (PDE), which gives us access to the full waveform inversion technique, usable in harmonic or temporal regime. The methods that we want to use are attractive because the weekly depend on the chosen criterion, and they are easily adaptable to various physical situations (multimodal decomposition in the pipe, coupling with the embouchure, ...), which can therefore be modified a posteriori. The goal is to proceed iteratively between instrument making and optimal design (the virtual workshop) in order to get close to tone quality related and playability criteria.

6.2.5. Energy based model and simulation in the time domain of linear acoustic waves in a radiating pipe

Participants: Juliette Chabassier, Robin Tournemenne.

We model in the time domain linear acoustic waves in a radiating pipe without damping. The acoustic equations system is formulated in flow and pressure, which leads to a first order space time equations system. The radiation condition is also written as a first order in time equation, and is parametrized by two real coefficients. Moreover, an auxiliary variable is introduced at the radiating boundary. The choice of this variable is adapted to the considered source type in order to ensure the model stability by energy techniques, under some conditions on the radiating condition. We then propose a stable space time explicit discretization, which ensures the dissipation of a discrete energy. The novelty of the discretization lies, on the one hand, in the variational nature of the space approximation (which leads to arbitrary order finite elements with no required matrix inversion), and on the other hand, on the definition of the auxiliary variable for any acoustic source type (which leads to the decay of a well defined energy). Finally, we quantify the frequential domain of validity of the used radiation condition by comparison with theoretical and experimental models of the literature. This is a collaboration with Morgane Bergot (Université Claude Bernard, Lyon 1).

6.2.6. Computation of the entry impedance of a dissipative radiating pipe

Participants: Juliette Chabassier, Robin Tournemenne.

Modeling the entry impedance of wind instruments pipes is essential for sound synthesis or instrument qualification. We study this modeling with the finite elements method in one dimension (FEM1D) and with the more classically used transfer matrix method (TMM). The TMM gives an analytical formula of the entry impedance depending on the bore (intern geometry of the instrument) defined as a concatenation of simple elements (cylinders, cones, etc). The FEM1D gives the entry impedance for any instrument geometry. The main goals of this work are to assess the viability of the FEM1D and to study the approximations necessary for the TMM in dissipative pipes. First, lossless Weber’s equation in one dimension is studied with arbitrary radiation conditions. In this context and for cylinders or cones, the TMM is exact. We verify that the error made with FEM1D for fine enough elements is as small as desired. When we consider viscothermal losses, the TMM does not solve the classical Kirchhoff model because two terms are supposed constant. In order to overcome this model approximation, simple elements, on which are based the TMM, are decomposed into much smaller elements. The FEM1D does not necessitate any model approximation, and it is possible to show that it solves the dissipative equation with any arbitrarily small error. With this in hand, we can quantify the TMM model approximation error.

6.2.7. Hybrid discontinuous finite element approximation for the elasto-acoustics.

Participants: Hélène Barucq, Julien Diaz, Elvira Shishenina.

Discontinuous Finite Element Methods (DG FEM) have proven their numerical accuracy and flexibility. However, numerically speaking, the high number of degrees of freedom required for computation makes them more expensive, compared to the standard techniques with continuous approximation. Among the different variational approaches to solve boundary value problems there exists a distinct family of methods, based on the use of trial functions in the form of exact solutions of the governing equations. The idea was first proposed
by Trefftz in 1926, and since then it has been largely developed and generalized. By its definition, Trefftz-DG methods reduce numerical cost, since the vari- ational formulation contains the surface integrals only. Thus, it makes possible exploration of the meshes with different geometry, in order to create more realistic application. Trefftz-type approaches have been widely used for time-harmonic problems, while their implementation is still limited in time domain. The particularity of Trefftz-DG methods applied to the time-dependent formulations consists in the use of space-time meshes. Even though it creates another computational difficulty, due to a dense form of the matrix, which represents the global linear system, the inversion of the full "space-time" matrix can be reduced to the inversion of one block-diagonal matrix, which corresponds to the interactions in time. In the present work, we develop a theory for solving the coupled elasto-acoustic wave propagation system. We study well-posedness of the problem, based on the error estimates in mesh-dependent norms. We consider a space-time polynomial basis for numerical discretization. The obtained numerical results are validated with analytical solutions. Regarding the advantages of the method, following properties have been proven by the numerical tests: high flexibility in the choice of basis functions, better order of convergence, low dispersion. These results have been obtained in collaboration with Henri Calandra (TOTAL) and have been published in a research report [43]. A paper has been submitted and a second one is being prepared.

6.2.8. Construction of stabilized high-order hybrid Galerkin schemes.

Participants: Hélène Barucq, Aurélien Citrain, Julien Diaz.

We have compared the performance of Discontinuous Galerkin Methods and Spectral Element Methods on academic benchmark and on realistic geophysical model in two dimensions. We have shown that, for a given accuracy, SEM on quadrilateral meshes could be 10 times faster than DGm, which justifies our strategy to consider SEM wherever it is possible to use quadrilateral/hexahedral cells. These first results have been presented in Matthias conference. Then, we have considered the SEM/DG coupling proposed for electromagnetics in [78] and we have implemented it in our acoustics code. We are now analyzing the performance of this strategy and we are extending it to deal with elastodynamic and elasto-acoustic coupling. The following steps will be the extension of the analysis to 3D dimensional problems and the application to realistic test case. The main bottleneck is obviously to the definition of an efficient strategy to couple tetrahedra and hexahedra. Indeed, if in the 2D case, the edges of both triangles and quadrilaterals are all segments the faces of tetrahedra are triangle while the faces of hexahedra are quadrilaterals. Hence, in 2D it sufficed to define integration on segment, while in 3D it will be necessary to consider integration of various polygon resulting of the intersection of triangle and quadrilaterals. Once this strategy is defined and implemented, we expect to be able to reduce the computational of the platform that we develop jointly with Total by a factor between 5 and 10. These results have been obtained in collaboration with Henri Calandra (TOTAL) and Christian Gout (INSA Rouen).

6.2.9. Modeling of dissipative porous media.

Participants: Juliette Chabassier, Julien Diaz, Fatima Jabiri.

In this work we have considered the modeling of 1D acoustic wave propagation coupled with visco-thermal losses that occur in porous media. We have proposed a family of dissipative models from which we have been able to obtain a quasi-constant quality factor (which is an indicator of the dissipation as a function of the frequency). We have derived stability conditions on the parameters of the model thanks to an energy analysis and we have rewritten the problem of designing a quasi-constant quality factor as a constrained least-square optimization problem. The parameters to optimize are the parameters of the family of dissipative models and the constraints are the stability of the final model. We are now considering the extension of the family to more general formulations and to heterogeneous media, before tackling multidimensional problems. These results have been obtained during the Master internship of Fatima Jabiri, in collaboration with Sébastien Imperiale (Inria Project-Team M3DISIM)

6.2.10. Asymptotic models for the electric potential across a highly conductive casing.

Application to the field of resistivity measurements.

Participants: Hélène Barucq, Aralar Erdozain, Victor Péron.
A configuration that involves a steel-cased borehole is analyzed, where the casing that covers the borehole is considered as a highly conductive thin layer. Asymptotic techniques are presented as the suitable tool for deriving reduced problems capable of dealing with the numerical issues caused by the casing when applying the traditional numerical methods. The derivation of several reduced models is detailed by employing two different approaches, each of them leading to different classes of models. The stability and convergence of these models is studied and uniform estimates are proved. The theoretical orders of convergence are supported by numerical results obtained with the finite element method. We develop an application to the field of resistivity measurements. The second derivative of the potential which solves a reduced model has been employed to recover the resistivity of rock formations. These results are in accordance with an experiment of Kaufmann for the reference solution and have been obtained in collaboration with David Pardo (UPV/EHU).


Participants: Hélène Barucq, Aralar Erdozain, Victor Péron.

A transmission problem for the electric potential is considered, where one part of the domain is a high-conductive casing. Semi-analytical solutions are derived for several asymptotic models. These asymptotic models are designed to replace the casing by appropriate impedance conditions in order to avoid numerical instabilities. A decomposition in Fourier series of the solution to these asymptotic models is characterized. As an application we reproduced successfully the experiment of Kaufmann, using his same parameters, but computing with a fourth order asymptotic model. This experiment allows to recover the resistivity of rock formations employing a second derivative of the potential along the vertical direction. These results have been obtained in collaboration with Ignacio Muga (Pontificia Universidad Catolica of Valparaiso).


Participants: Justine Labat, Victor Péron, Sébastien Tordeux.

In the context of non-destructive testing in medical imaging or civil engineering, the detection of small heterogeneities can be a difficult task in three dimensional domains. The complexity for solving numerically the direct problem both in terms of computation time and memory cost is due to the small size of obstacles in comparison with the incident wavelength and the large size of the domain of interest. Then the fine mesh size makes unsuitable or too expensive the use of classical numerical methods type continuous and discontinuous finite element methods or boundary element methods. The use of reduced models allows to get an approximation of the exact solution at a certain accuracy with a lower cost. We develop a Matched Asymptotic Expansions method to solve a time-harmonic electromagnetic scattering problem by a small sphere. This method allows to replace the scatterer by an equivalent asymptotic point source. In practice, it consists in defining an approximate solution using multi-scale expansions over far and near fields, related in a matching area. When the scatterer is a sphere, we make explicit the asymptotic expansions until the second order of approximation, relatively to the sphere radius. Numerical results make evident the convergence rate with respect to the sphere radius. Reference solutions are analytical solutions computed thanks to Montjoie Code. This work has been presented in the Caleta Numerica seminar, Pontificia Universidad Catolica of Valparaiso, Chili [48].


Participant: Victor Péron.

This work is concerned with the time-harmonic eddy current problem for a medium with a highly conductive thin sheet. We present asymptotic models and impedance conditions up to the second order of approximation for the electromagnetic field. The conditions are derived asymptotically for vanishing sheet thickness $\varepsilon$ where the skin depth is scaled like $\varepsilon$. The first order condition is the perfect electric conductor boundary condition. The second order condition turns out to be a Poincaré-Steklov map between tangential components of the magnetic field and the electric field [49]. Numerical experiments have been performed to assess the accuracy.
of the second order model. Complementary simulations will be conducted to study the robustness with respect to the sheet conductivity and the convergence of the modelling error. These results have been obtained in collaboration with Mohammad Issa and Ronan Perrussel (LAPLACE, CNRS/IMPT/UPS, Univ. de Toulouse) and this work has been presented in the international conference ACOMEN 2017 [33].


Participants: Hélène Barucq, Juliette Chabassier, Ha Pham, Sébastien Tordeux.

We investigate efficient methods to simulate the multiple scattering of obstacles in homogeneous media. With a large number of small obstacles on a large domain, optimized pieces of software based on spatial discretization such as Finite Element Method (FEM) or Finite Difference lose their robustness. As an alternative, we work with an integral equation method, which uses single-layer potentials and truncation of Fourier series to describe the approximate scattered field. In the theoretical part of the paper, we describe in detail the linear systems generated by the method for impenetrable obstacles, accompanied by a well-posedness study. For the numerical performance study, we limit ourselves to the case of circular obstacles. We first compare and validate our codes with the highly optimized FEM-based software Montjoie. Secondly, we investigate the efficiency of different solver types (direct and iterative of type GMRES) in solving the dense linear system generated by the method. We observe the robustness of direct solvers over iterative ones for closely-spaced obstacles, and that of GMRES with Lower–Upper Symmetric Gauss–Seidel and Symmetric Gauss–Seidel preconditioners for far-apart obstacles.

This work has been published in the journal Wave Motion, [15] and is also connected to the following conference presentations, [31], [41].

6.2.15. A study of the Numerical Dispersion for the Continuous Galerkin discretization of the one-dimensional Helmholtz equation

Participants: Hélène Barucq, Ha Pham, Sébastien Tordeux.

This work is a collaboration with Henri Calandra (TOTAL).

Although true solutions of Helmholtz equation are non-dispersive, their discretizations suffer from a phenomenon called numerical dispersion. While the true phase velocity is constant, the numerical one changes with the discretization scheme, order and mesh size. In our work, we study the dispersion associated with classical finite element. For arbitrary order of discretization, without using an Ansatz, we construct the numerical solution on the whole \( \mathbb{R} \), and obtain an asymptotic expansion for the phase difference between the exact wavenumber and the numerical one. We follow an approach analogous to that employed in the construction of true solutions at positive wavenumbers, which involves Z-transform, contour deformation and limiting absorption principle. This perspective allows us to identify the numerical wavenumber with the angle of analytic poles. Such an identification is useful since the latter (analytic poles) can be numerically evaluated by an algorithm, which then yields the value of numerical wavenumber.

This work is detailed in the research report [44].

6.3. Supercomputing for Helmholtz problems

6.3.1. Numerical libraries for hybrid meshes in a discontinuous Galerkin context

Participants: Hélène Barucq, Lionel Boillot, Aurélien Citrain, Julien Diaz.

Elasticus team code has been designed for triangles and tetrahedra mesh cell types. The first part of this work was dedicated to add quadrangle libraries and then to extend them to hybrid triangles-quadrangles (so in 2D). This implied to work on polynomials to form functions basis for the (discontinuous) finite element method, to finally be able to construct reference matrices (mass, stiffness, ...).
A complementary work has been done on mesh generation. The goal was to encircle an unstructured triangle mesh, obtained by third-party softwares, with a quadrangle mesh layer. At first, we built scripts to generate structured triangle meshes, quadrangle meshes and hybrid meshes (triangles surrounded by quadrangles). We are now able to couple unstructured triangle mesh with structured quadrangle mesh, and we are now working on the implementation of the coupling between Discontinuous Galerkin methods (for the triangles) and Spectral Element methods (for the quadrangles).

6.3.2. *Hybridizable Discontinuous Galerkin methods for solving the elastic Helmholtz equations*

**Participants:** Marie Bonnasse-Gahot, Julien Diaz.

The advantage of performing seismic imaging in frequency domain is that it is not necessary to store the solution at each time step of the forward simulation. Unfortunately, the drawback of the Helmholtz equations, when considering 3D realistic elastic cases, lies in solving large linear systems. This represents today a challenging task even with the use of High Performance Computing (HPC). To reduce the size of the global linear system, we developed a Hybridizable Discontinuous Galerkin method (HDGm). It consists in expressing the unknowns of the initial problem in function of the trace of the numerical solution on each face of the mesh cells. In this way the size of the matrix to be inverted only depends on the number of degrees of freedom on each face and on the number of the faces of the mesh, instead of the number of degrees of freedom on each cell and on the number of the cells of the mesh as we have for the classical Discontinuous Galerkin methods (DGm). The solution to the initial problem is then recovered thanks to independent elementwise calculation. These results have been published in [18]. This is a collaboration with Henri Calandra (Total) and Stéphane Lanteri (Inria Project Team Nachos).

6.3.3. *Scalability of linear solvers for Hybridizable Discontinuous Galerkin methods*

**Participants:** Marie Bonnasse-Gahot, Julien Diaz.

We coupled our HDG code with tested two linear solvers: a parallel sparse direct solver MUMPS (MUltifrontal Massively Parallel sparse direct Solver) and a hybrid solver MaPHyS (Massively Parallel Hybrid Solver) which combines direct and iterative methods. In the framework of the european project HPC4E, we analyzed the scalability of the two solvers on the plateform Plafrim. We compared the performances of the two solvers when solving 3D elastic waves propagation over HDGm. These comparisons were presented at the 2017 EAGE Workshop on High Performance Computing for Upstream and at MATHIAS 2017 conferences. This is a collaboration with Henri Calandra (Total), Luc Giraud, Mathieu Kuhn (Inria Project-Team Hiepacs) and Stéphane Lanteri (Inria Project Team Nachos).

6.4. *Hybrid time discretizations of high-order*

6.4.1. *Construction and analysis of a fourth order, energy preserving, explicit time discretization for dissipative linear wave equations.*

**Participants:** Juliette Chabassier, Julien Diaz, Anh-Tuan Ha.

We submitted a paper to M2AN. This paper deals with the construction of a fourth order, energy preserving, explicit time discretization for dissipative linear wave equations. This scheme is obtained by replacing the inversion of a matrix, that comes naturally after using the technique of the Modified Equation on the second order Leap Frog scheme applied to dissipative linear wave equations, by an explicit approximation of its inverse. The stability of the scheme is studied first using an energy analysis, then an eigenvalue analysis. Numerical results in 1D illustrate the good behavior regarding space/time convergence and the efficiency of the newly derived scheme compared to more classical time discretizations. A loss of accuracy is observed for non smooth profiles of dissipation, and we propose an extension of the method that fixes this issue. Finally, we assess the good performance of the scheme for a realistic dissipation phenomenon in Lorentz’s materials. This work has been done in collaboration with Sébastien Imperiale (Inria Project-Team M3DISIM) and Alain Anh-Tuan Ha (Internship at Magique 3D in 2016).
6.4.2. Higher-order optimized explicit Runge-Kutta schemes for linear ODEs  
**Participants:** Hélène Barucq, Marc Duruflé, Mamadou N’Diaye.

In this work, we have constructed optimized explicit Runge-Kutta schemes for linear ODEs that we called Linear-ERK. Theses schemes can be applied to the following ODE

\[ M_h \frac{dU}{dt} = K_h U + F(t) \]

where \( M_h \) is the mass matrix, \( K_h \) the stiffness matrix and \( F(t) \) a source term. Linear-ERK schemes are constructed using polynomial stability functions which are obtained by maximizing the CFL number. We have considered a polynomial stability function based on the Taylor series expansion of an exponential function. Then, we have added extra terms beyond the terms of the Taylor expansion without changing the order of accuracy. The coefficients of those extra terms have been computed by optimizing the CFL number such that the stability region of the developed scheme includes a typical spectrum. This spectrum has been obtained by computing eigenvalues of the matrix \( M_h^{-1} K_h \) for the wave equation solved on a square with Hybrid Discontinuous Formulation (HDG). The optimization is performed by using the algorithm developed by D. Ketcheson and coworkers. By proceeding this way, we have obtained optimized explicit schemes up to order 8.

We have also determined the CFL number and the efficiency on the typical spectrum for each explicit scheme. We have provided algorithms to implement these schemes and numerical results to compare them.

This work is a chapter of the thesis defended by Mamadou N’diaye on December 8, 2017, under the joint supervision of Hélène Barucq and Marc Duruflé.

6.4.3. High-order locally implicit time schemes for linear ODEs  
**Participants:** Hélène Barucq, Marc Duruflé, Mamadou N’Diaye.

In this work we have proposed a method that combines optimized explicit schemes and implicit schemes to form locally implicit schemes for linear ODEs, including in particular ODEs coming from the space discretization of wave propagation phenomena. This method can be applied to the following ODE

\[ M_h \frac{dU}{dt} = K_h U + F(t) \]

Like in the local time-stepping developed by Grote and co-workers, the computational domain is split into a fine region and a coarse region. The matrix \( A_h \) is given as

\[ A_h = M_h^{-1} K_h = A_h P + A_h (I - P) \]

where \( P \) is the projector on the fine region of the computational domain. Then the proposed locally implicit method is obtained from the combination of the A-stable implicit schemes we have developed in 2016 (Padé schemes or Linear-SDIRK schemes detailed in [17]) on the fine region and explicit schemes with optimal CFL number in the coarse region. The developed method has been used to solve the acoustic wave equation and we have checked the convergence in time of these schemes for order 4, 6 and 8.

This work has been presented at the Mathias annual Total seminar and is a chapter of the thesis defended by Mamadou N’diaye on December 8, 2017, under the joint supervision of Hélène Barucq and Marc Duruflé.
7. Bilateral Contracts and Grants with Industry

7.1. Contracts with TOTAL

- Depth Imaging Partnership (DIP)
- Approximations hybrides par éléments finis discontinus pour l’élasto-acoustique
- Méthodes d’inversion sismique dans le domaine fréquentiel
- Portage de méthodes numériques de simulation de phénomènes complexes sur des architectures exascales
- Utilisation d’images 3D DRP à différentes échelles et résolutions pour vérifier l’applicabilité des problèmes acoustiques
- Petrophysics in pre-salt carbonate rocks

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. Partnership with I2M in Bordeaux supported by Conseil Régional d’Aquitaine

Title: Imaging complex materials.
Coordinator: Hélène Barucq
Other partners: I2M CNRS Université Bordeaux I

The detection, localization and monitoring of the defect evolution in composite materials, concrete and more generally heterogeneous materials is a challenging problem for Aeronautics and energy production. It is already possible to localize defects in homogeneous materials by using methods based on ultrasonic inspection and sometimes, they are usable in particular heterogeneous materials, most of the time in 2D. Classical methods rely on the correspondence between the distance and the propagation time of the wave traveling between the defect and the receivers. In complex media, such a correspondence may be lapsed, for instance when the velocity depends on the frequency (dispersion) or of the propagation direction (anisotropy). The defect signature can also be embedded in the acoustic field sent by the structure (multiple reflections). The complexity of the propagation in heterogeneous materials makes then difficult the accurate localization of the defect, in particular in 3D.

Topological imaging techniques can be applied to heterogeneous media. They can find the positions of defects from two simulations performed in a safe experimental medium. They have been developed at I2M laboratory to carry on 2D single/multi mode inspection in isotropic and anisotropic waveguides. They have also been applied to a highly reflecting medium observed with a single sensor. The objective of this work is to extend the technique to 3D problems. In particular, we are going to handle detection in composite plates and in highly heterogeneous media including a collection of small scatterers.
This project is supported by the Conseil Régional d’Aquitaine, for a duration of 2 years.

8.2. National Initiatives

8.2.1. Depth Imaging Partnership

Magique-3D maintains active collaborations with Total. In the context of Depth Imaging, Magique-3D coordinates research activities dealing with the development of high-performance numerical methods for solving wave equations in complex media. This project has involved 2 other Inria Team-Projects (Hiepacs and Nachos) which have complementary skills in mathematics, computing and in geophysics. DIP is fully funded by Total by the way of an outline agreement with Inria.

In 2014, the second phase of DIP has begun. Lionel Boillot has been hired as engineer to work on the DIP platform. Six PhD students have defended their PhD since 2014 and they are now post-doctoral researchers or engineers in Europe. DIP is currently employing 2 PhD students and one post-doctoral researcher.

8.2.2. ANR Num4Sun

The ANR has launched a specific program for supporting and promoting applications to European or more generally International projects. Magique-3D has been selected in 2016 after proposing a project to be applied as a FET project on the occasion of a call that will open in 2017 April. This project will gather researchers of the MPS (https://www.mps.mpg.de/en), of the BSC (https://www.bsc.es/), of the BCAM (http://www.bcamath.org/en/), of Heriot-Watt University (https://www.hw.ac.uk/) and Inria teams.

A kick-off meeting has been held in November 2016 in Strasbourg and a second one in Paris in July 2017. Thanks to this support, we have submitted a ETPHPC proposal in September 2017 The project is funded for 18 months starting from August 2016. The funding amounts 30000€.

8.2.3. ANR NonLocalDD

Magique 3-D is a partner of the ANR project entitled "Non Local Domain Decomposition Methods in Electromagnetics" that begins in october 2015. The aim of this project is to develop domain decomposition methods for the efficient solution of acoustics and Maxwell’s equation either with boundary integral equations or finite element volume method. To obtain an exponential convergence of the iterative solution, non-local operators are studied and optimized to achieve a faster convergence. A post-doctoral student Marcella Bonazzoli has been hired by Magique 3-D in 2017 to study multi-domain integral equations for wave propagation. This student is supervised by Xavier Claeys, a partner of the NonLocalDD ANR project.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. GEAGAM

Title: Geophysical Exploration using Advanced GAllerkin Methods
Program: H2020
Duration: January 2015 - December 2017
Coordinator: Universidad Del Pais Vasco (EHU UPV)
Partners:
Beam - Basque Center for Applied Mathematics Asociacion (Spain)
Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)
Total S.A. (France)
Universidad Del Pais Vasco Ehu Upv (Spain)
Pontificia Universidad Catolica de Valparaiso (Chile)
Universidad de Chile (Chile)
The main objective of this Marie Curie RISE action is to improve and exchange interdisciplinary knowledge on applied mathematics, high performance computing, and geophysics to be able to better simulate and understand the materials composing the Earth’s subsurface. This is essential for a variety of applications such as CO2 storage, hydrocarbon extraction, mining, and geothermal energy production, among others. All these problems have in common the need to obtain an accurate characterization of the Earth’s subsurface, and to achieve this goal, several complementary areas will be studied, including the mathematical foundations of various high-order Galerkin multiphysics simulation methods, the efficient computer implementation of these methods in large parallel machines and GPUs, and some crucial geophysical aspects such as the design of measurement acquisition systems in different scenarios. Results will be widely disseminated through publications, workshops, post-graduate courses to train new researchers, a dedicated webpage, and visits to companies working in the area. In that way, we will perform an important role in technology transfer between the most advanced numerical methods and mathematics of the moment and the area of applied geophysics.

8.3.1.2. HPC4E

Title: HPC for Energy
Program: H2020
Duration: December 2015 - November 2017
Coordinator: Barcelona Supercomputing Center
Partners:

- Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas-Ciemat (Spain)
- Iberdrola Renovables Energia (Spain)
- Repsol (Spain)
- Lancaster University (United Kingdom)
- Total S.A. (France)
- Fundação Coordenação de Projetos, Pesquisas e Estudos Tecnológicos, (Brazil)
- National Laboratory for Scientific Computation, (Brazil)
- Instituto Tecnológico de Aeronáutica, (Brazil)
- Petrobras, (Brazil)
- Universidade Federal do Rio Grande do Sul, (Brazil)
- Universidade Federal de Pernambuco, (Brazil)

Inria contact: Stéphane Lanteri

This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO2 emissions, contribution to diversification of energy
supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial applications using alternative fuels, which is required to design efficient furnaces, engines, clean burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth’s interior with unprecedented quality.

8.4. International Initiatives

8.4.1. Inria International Partners

8.4.1.1. Declared Inria International Partners

8.4.1.1.1. MAGIC2

Title: Advance Modeling in Geophysics

International Partner (Institution - Laboratory - Researcher):

California State University at Northridge (United States) - Department of Mathematics - Djellouli Rabia

The Associated Team MAGIC was created in January 2006 and renewed in January 2009. At the end of the program in December 2011, the two partners, MAGIQUE-3D and the California State University at Northridge (CSUN) decided to continue their collaboration and obtained the “Inria International Partner” label in 2013.

See also: https://project.inria.fr/magic/

The ultimate objective of this research collaboration is to develop efficient solution methodologies for solving inverse problems arising in various applications such as geophysical exploration, underwater acoustics, and electromagnetics. To this end, the research program will be based upon the following three pillars that are the key ingredients for successfully solving inverse obstacle problems. 1) The design of efficient methods for solving high-frequency wave problems. 2) The sensitivity analysis of the scattered field to the shape and parameters of heterogeneities/scatterers. 3) The construction of higher-order Absorbing Boundary Conditions.

In the framework of Magic2, Izar Azpiroz visited CSUN in May 2017 and Rabia Djellouli (CSUN) visited Magique 3D in December 2017

8.5. International Research Visitors

8.5.1. Visits of International Scientists

• Rabia Djellouli (CSUN) visited Magique 3D in December 2017.
• Damien Fournier (MPS) visited Magique 3D in October 2017.
• Morgane Bergot (Univ Lyon) visited Magique 3D in November 2017.

8.5.2. Visits to International Teams

8.5.2.1. Research Stays Abroad

• In the framework of the European project Geagam, Izar Azpiroz and Justine Labat visited Ignacio Muga, PUCV, Chile, in April 2017.
• In the framework of the International Partnership Magic2, Izar Azpiroz visited Rabia Djellouli, CSUN (California State University at Northridge), USA, in May 2017.
9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

- Hélène Barucq, Julien Diaz and Sébastien Tordeux organized the conference in honor of Abderrahmane Bendali in Pau, December 12th-14th, 2017, https://project.inria.fr/bendali/
- Julien Diaz co-organized the conference in honor of Patrick Joly in Saclay, August 28th-30th 2017, in Saclay https://wavesjoly60.inria.fr/

9.1.1.2. Member of the Conference Program Committees

- Hélène Barucq and Julien Diaz were members of the scientific committee of Waves 2017 https://cceevents.umn.edu/waves-2017

9.1.2. Journal

9.1.2.1. Reviewer - Reviewing Activities

Members of Magique 3D have been reviewers for the following journals:

- Applied Numerical Mathematics
- Mathematics and Computers in Simulation
- International Journal for Numerical Methods in Engineering
- Geophysical Journal International
- IMA Journal of Numerical Analysis
- SIAM Journal on Scientific Computing
- Computers and Mathematics with Applications
- Journal of Mathematical Analysis and Applications
- Journal of Computational Physics
- Journal of the Acoustical Society of America

9.1.3. Scientific Expertise

- Julien Diaz was expert for the evaluation of Millennium Science Initiative project for the government of Chile.

9.1.4. Research Administration

- Hélène Barucq has been the chairwoman of the local jury of Inria competitive selection for Young Graduate Scientists (CR2) in Bordeaux. She has been part of a working group dealing with the new strategic plan of Inria. In January 2017, she has been appointed chairwoman of the committee created by the regional council of Nouvelle Aquitaine. She is in charge of the scientific evaluation of research projects in Mathematics, Informatics, Electronics, Optics. She is the scientific head of the project DIP since its creation in 2009.
- Juliette Chabassier is member of the Inria BSO Young Researcher Committee and of the Inria BSO Center Committee. She is member of the Workgroup for sustainable development at Inria Bordeaux Sud-Ouest.
- Julien Diaz is elected member of the Inria Technical Committee and of the Inria Administrative ans Scientific Boards. He is appointed member of the CDT (Commission de Développement Technologique)
- Mamadou N’Diaye is member of the Center Committee of Inria Bordeaux Sud-Ouest.
Victor Péron is appointed member of the CJC (Commission Jeunes Chercheurs) of Inria Bordeaux Sud-Ouest.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Master : Julien Diaz, Transformées, 24h Eq. TD, M1, EISTIA, France
Licence : Justine Labat, Algèbre 1, 19,5h Eq. TD, L1, UPPA, France
Licence : Justine Labat, Algèbre linéaire, 19,5h Eq. TD, L1, UPPA, France
Licence : Justine Labat, Introduction aux Probabilités, 19,5h Eq. TD, L2, UPPA, France
Licence : Victor Péron, Analyse 2, 39 Eq. TD, L1, UPPA, France
Licence : Victor Péron, Mathématiques appliquées, 15 Eq. TD, L1, UPPA, France
Licence : Victor Péron, Courbes et calcul intégral, 19.5 Eq. TD, L2, UPPA, France
Licence : Victor Péron, Analyse numérique des systèmes lin., 48.75 Eq. TD, L3, UPPA, France
Master : Victor Péron et Sébastien Tordeux, Analyse num. des EDP 1: différences finies, 75 eq. TD, Master1, UPPA, FRANCE
Master : Victor Péron et Sébastien Tordeux, Introduction aux phénomènes de propagation d’ondes, 38 eq. TD, Master 2, UPPA, FRANCE
Master : Victor Péron et Sébastien Tordeux, Méthodes asymptotiques, 35 eq. TD, Master 2, UPPA, FRANCE

9.2.2. Supervision

PhD : Vincent Darrigrand, Étude d’erreur pour des problèmes d’Helmholtz approchés par des techniques de Petrov-Galerkin, September 1st 2017, Hélène Barucq and David Pardo.
PhD : Florian Faucher, Méthodes d’inversion sismique dans le domaine fréquentiel, November 29th 2017, Hélène Barucq.
PhD : Mamadou N’Diaye, Analyse et développement de schémas temporels hybrides pour les équations hyperboliques du premier ordre, December 8th 2017, Hélène Barucq and Marc Duruflé.
PhD in progress : Aurélien Citrain, Déformation 3D de maillages en imagerie sismique, Méthodes d’inversion sismique dans le domaine fréquentiel, October 2016, Hélène Barucq and Christian Gout.
PhD in progress : Izar Azpiroz Iragorri, Approximation des problèmes d’Helmholtz couplés sur maillages virtuels, October 2014, Hélène Barucq, Julien Diaz and Rabia Djellouli (CSUN).
PhD in progress : Justine Labat, Diffraction of an electromagnetic wave by small obstacles, Université de Pau et des Pays de l’Adour, October 2016, Victor Péron and Sébastien Tordeux
PhD in progress : Hamza Alaoui Hafidi, Imagerie ultrasonore tridimensionnelle dans les milieux hétérogènes complexes, October 2015, Encadrement : Marc Deschamps, Michel Castaings, Eric Ducasse, Samuel Rodriguez (I2M), Hélène Barucq, Marc Duruflé, Juliette Chabassier (Magique 3D).
PhD in progress : Pierre Jacquet, ,October 2015, Hélène Barucq and Julien Diaz.
PhD in progress : Chengyi Shen, Approches expérimentale et numérique de la propagation d’ondes sismiques dans les roches carbonatées, October 2016, Julien Diaz and Daniel Brito (LFC).
PhD in progress : Elvira Shishenina, Approximations hybrides par éléments finis et éléments virtuels discontinus pour l’élasto-acoustique, October 2015, Hélène Barucq and Julien Diaz.
PhD in progress : Alexandre Gras, Hybrid resonance for sensing applications, IOGS, October 2017, 
Encadrement : Philippe Lalanne (IOGS), Marc Duruflé, Hélène Barucq (Magique 3D) 
Master 1 internship : Kevin Lagnoux, Détermination des paramètres physiques et de forme d’un 
Master 1 internship : Fatima Ezzahra, Formulation de modèles de dissipation dans les milieux poreux 

9.2.3. Juries

- Hélène Barucq : Laure Pesudo (Université Paris Saclay) "Une méthode hybride couplant la méthode 
des équations intégrales et la méthode des rayons en vue d’applications au contrôle non destructif 
ultrasonore", PhD thesis, October 8th 2017
- Hélène Barucq : Victor Péron (Université de Pau et des Pays de l’Adour) "Analyse asymptotique et 
calcul scientifique pour des applications en physique", HDR, December 6th 2017
- Hélène Barucq (reviewer): Sébastien Pernet (Université Paul Sabatier, Toulouse) "Quelques méth-
odes performantes pour la simulation des phénomènes de propagation et de diffraction d’ondes", 
HDR, December 11th 2017
- Hélène Barucq (reviewer): Marius Albrand (Université Paul Sabatier, Toulouse) "Étude d’une 
solution d’évaluation des constantes diélectriques du béton d’ouvrages à risque par une approche 
problème inverse en électromagnétisme", PhD thesis, December 18th 2017
- Julien Diaz (reviewer): Mohamed Lakhal (Université Paris Saclay) "Méthodes d’inversion pour la 
reconstruction de mines enfouies à partir de mesures d’antennes radar.", PhD thesis, June 22nd 2017
- Julien Diaz : Vincent Darrigrand (University of Basque Country/Université de Pau et des Pays 
de l’Adour) "Goal-oriented adaptivity using unconventional error representations", PhD thesis, 
September 1st 2017
- Julien Diaz : Octavio Castillo Reyes (UPC Universitat Politecnica de Catalunya) "Edge-Elements 
- Julien Diaz : Mamadou N’Diaye (Université de Pau et des Pays de l’Adour) "Étude et développement 
de méthodes numériques d’ordre élevé pour la résolution des équations différentielles ordinaires 
(EDO), applications à la résolution des équations d’ondes acoustiques et électromagnétiques.", PhD 
thesis, December 8th 2017
- Juliette Chabassier : Jin Jack Tan (Université Paris Saclay) “Piano acoustics: string’s double polari-

9.3. Popularization

- Juliette Chabassier shared her experience as a scientist in the collège de Lussac in March 2017.
- Juliette Chabassier participated in scientific “speed datings” during the “Filles et Maths” day in April 
2017.
- Juliette Chabassier shared her experience as a scientist during “Printemps de la Mixité” in May 
2017.
- Juliette Chabassier presented a talk around mathematics in music in Pau in April 2017.
- Juliette Chabassier co-organized a series of three conferences around the theme of women in 
informatics in 2017.
- Juliette Chabassier gave a talk about mathematics in music in Bordeaux during the "découvreuses 
anonymes" exposition in November 2017.
- Juliette Chabassier gave a pitch of science during the national event "50 ans Inria" in November 
2017.
10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


[22] D. Fournier, M. Leguèbe, C. S. Hanson, L. Gizon, H. Barucq, J. Chabassier, M. Duruflé.Atmospheric radiation boundary conditions for high frequency waves in time-distance helioseismol-
Activity Report INRIA 2017


Invited Conferences


International Conferences with Proceedings


the Project Review, Geo-Mathematical Imaging Group at Rice University, Houston TX”, Houston, TX, United States, Proceedings of the Project Review, Geo-Mathematical Imaging Group at Rice University, Houston TX, Proceedings of the Project Review, Geo-Mathematical Imaging Group at Rice University, Houston TX, April 2017, vol. 1, p. 31–42, https://hal.archives-ouvertes.fr/hal-01623949.


Conferences without Proceedings


Research Reports


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Project-Team MANAO

Melting the frontiers between Light, Shape and Matter

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI), Laboratoire Photonique, Numérique et Nanosciences (LP2N)

IN PARTNERSHIP WITH:
CNRS
Institut d’Optique Graduate School
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Interaction and visualization
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Project-Team MANAO

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- A5.5. - Computer graphics
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- A5.5.3. - Computational photography
- A5.5.4. - Animation
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- A6.2.5. - Numerical Linear Algebra
- A6.2.6. - Optimization
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- B9.2.3. - Video games
- B9.5. - Humanities
- B9.5.6. - Archeology, History
- B9.5.10. - Digital humanities

1. Personnel

**Research Scientists**
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- Gaël Guennebaud [Inria, Researcher]

**Faculty Members**
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- Pierre Bénard [Univ. Bordeaux, Associate Professor]
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**External Collaborators**
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2. Overall Objectives

2.1. General Introduction

Computer generated images are ubiquitous in our everyday life. Such images are the result of a process that has seldom changed over the years: the optical phenomena due to the propagation of light in a 3D environment are simulated taking into account how light is scattered [58], [36] according to shape and material characteristics of objects. The intersection of optics (for the underlying laws of physics) and computer science (for its modeling and computational efficiency aspects) provides a unique opportunity to tighten the links between these domains in order to first improve the image generation process (computer graphics, optics and virtual reality) and next to develop new acquisition and display technologies (optics, mixed reality and machine vision).

Most of the time, light, shape, and matter properties are studied, acquired, and modeled separately, relying on realistic or stylized rendering processes to combine them in order to create final pixel colors. Such modularity, inherited from classical physics, has the practical advantage of permitting to reuse the same models in various contexts. However, independent developments lead to un-optimized pipelines and difficult-to-control solutions since it is often not clear which part of the expected result is caused by which property. Indeed, the most efficient solutions are most often the ones that blur the frontiers between light, shape, and matter to lead to specialized and optimized pipelines, as in real-time applications (like Bidirectional Texture Functions [68] and Light-Field rendering [34]). Keeping these three properties separated may lead to other problems. For instance:

- Measured materials are too detailed to be usable in rendering systems and data reduction techniques have to be developed [66], [69], leading to an inefficient transfer between real and digital worlds;
It is currently extremely challenging (if not impossible) to directly control or manipulate the interactions between light, shape, and matter. Accurate lighting processes may create solutions that do not fulfill users’ expectations;

- Artists can spend hours and days in modeling highly complex surfaces whose details will not be visible [89] due to inappropriate use of certain light sources or reflection properties.

Most traditional applications target human observers. Depending on how deep we take into account the specificity of each user, the requirement of representations, and algorithms may differ.

![Image](image.png)

**Figure 1. Examples of new display technologies. Nowadays, they are not limited to a simple array of 2D low-dynamic RGB values.**

With the evolution of measurement and display technologies that go beyond conventional images (e.g., as illustrated in Figure 1, High-Dynamic Range Imaging [79], stereo displays or new display technologies [54], and physical fabrication [25], [42], [50]) the frontiers between real and virtual worlds are vanishing [38]. In this context, a sensor combined with computational capabilities may also be considered as another kind of observer. Creating separate models for light, shape, and matter for such an extended range of applications and observers is often inefficient and sometimes provides unexpected results. Pertinent solutions must be able to take into account properties of the observer (human or machine) and application goals.

### 2.2. Methodology

![Diagram](diagram.png)

**Figure 2. Interactions/Transfers between real and virtual worlds. One of our goal is to combine optical instruments with processes from computer science in order to blend the two worlds.**

#### 2.2.1. Using a global approach

The main goal of the MANAO project is to study phenomena resulting from the interactions between the three components that describe light propagation and scattering in a 3D environment: light, shape, and matter. Improving knowledge about these phenomena facilitates the adaption of the developed digital, numerical, and analytic models to specific contexts. This leads to the development of new analysis tools, new representations, and new instruments for acquisition, visualization, and display.
To reach this goal, we have to first increase our understanding of the different phenomena resulting from the interactions between light, shape, and matter. For this purpose, we consider how they are captured or perceived by the final observer, taking into account the relative influence of each of the three components. Examples include but are not limited to:

- The manipulation of light to reveal reflective [31] or geometric properties [95], as mastered by professional photographers;
- The modification of material characteristics or lighting conditions [96] to better understand shape features, for instance to decipher archaeological artifacts;
- The large influence of shape on the captured variation of shading [77] and thus on the perception of material properties [92].

Based on the acquired knowledge of the influence of each of the components, we aim at developing new models that combine two or three of these components. Examples include the modeling of Bidirectional Texture Functions (BTFs) [41] that encode in a unique representation effects of parallax, multiple light reflections, and also shadows without requiring to store separately the reflective properties and the meso-scale geometric details, or Light-Fields that are used to render 3D scenes by storing only the result of the interactions between light, shape, and matter both in complex real environments and in simulated ones.

One of the strengths of MANAO is that we are inter-connecting computer graphics and optics. On one side, the laws of physics are required to create images but may be bent to either increase performance or user’s control: this is one of the key advantages of computer graphics approach. It is worth noticing that what is not possible in the real world may be possible in a digital world. However, on the other side, the introduced approximations may help to better comprehend the physical interactions of light, shape, and matter.

2.2.2. Taking observers into account

The MANAO project specifically aims at considering information transfer, first from the real world to the virtual world (acquisition and creation), then from computers to observers (visualization and display). For this purpose, we use a larger definition of what an observer is: it may be a human user or a physical sensor equipped with processing capabilities. Sensors and their characteristics must be taken into account in the same way as we take into account the human visual system in computer graphics. Similarly, computational capabilities may be compared to cognitive capabilities of human users. Some characteristics are common to all observers, such as the scale of observed phenomena. Some others are more specific to a set of observers. For this purpose, we have identified two classes of applications.

- Physical systems Provided our partnership that leads to close relationships with optics, one novelty of our approach is to extend the range of possible observers to physical sensors in order to work on domains such as simulation, mixed reality, and testing. Capturing, processing, and visualizing complex data is now more and more accessible to everyone, leading to the possible convergence of real and virtual worlds through visual signals. This signal is traditionally captured by cameras. It is now possible to augment them by projecting (e.g., the infrared laser of Microsoft Kinect) and capturing (e.g., GPS localization) other signals that are outside the visible range. These supplemental information replace values traditionally extracted from standard images and thus lower down requirements in computational power [65]. Since the captured images are the result of the interactions between light, shape, and matter, the approaches and the improved knowledge from MANAO help in designing interactive acquisition and rendering technologies that are required to merge the real and the virtual world. With the resulting unified systems (optical and digital), transfer of pertinent information is favored and inefficient conversion is likely avoided, leading to new uses in interactive computer graphics applications, like augmented reality [30], [38] and computational photography [78].

- Interactive visualization This direction includes domains such as scientific illustration and visualization, artistic or plausible rendering. In all these cases, the observer, a human, takes part in the process, justifying once more our focus on real-time methods. When targeting average users, characteristics as well as limitations of the human visual system should be taken into account: in
particular, it is known that some configurations of light, shape, and matter have masking and facilitation effects on visual perception [89]. For specialized applications, the expertise of the final user and the constraints for 3D user interfaces lead to new uses and dedicated solutions for models and algorithms.

3. Research Program

3.1. Related Scientific Domains

![Figure 3. Related scientific domains of the MANAO project.](image)

The MANAO project aims at studying, acquiring, modeling, and rendering the interactions between the three components that are light, shape, and matter from the viewpoint of an observer. As detailed more lengthily in the next section, such a work will be done using the following approach: first, we will tend to consider that these three components do not have strict frontiers when considering their impacts on the final observers; then, we will not only work in computer graphics, but also at the intersection of computer graphics and optics, exploring the mutual benefits that the two domains may provide. It is thus intrinsically a transdisciplinary project (as illustrated in Figure 3) and we expect results in both domains.

Thus, the proposed team-project aims at establishing a close collaboration between computer graphics (e.g., 3D modeling, geometry processing, shading techniques, vector graphics, and GPU programming) and optics (e.g., design of optical instruments, and theories of light propagation). The following examples illustrate the strengths of such a partnership. First, in addition to simpler radiative transfer equations [43] commonly used in computer graphics, research in the later will be based on state-of-the-art understanding of light propagation and scattering in real environments. Furthermore, research will rely on appropriate instrumentation expertise for the measurement [55], [56] and display [54] of the different phenomena. Reciprocally, optics researches may benefit from the expertise of computer graphics scientists on efficient processing to investigate interactive simulation, visualization, and design. Furthermore, new systems may be developed by unifying optical and digital processing capabilities. Currently, the scientific background of most of the team members is related to computer graphics and computer vision. A large part of their work have been focused on simulating and analyzing optical phenomena as well as in acquiring and visualizing them. Combined with the close collaboration with the optics laboratory LP2N (http://www.lp2n.fr) and with the students issued from the “Institut d’Optique” (http://www.institutoptique.fr), this background ensures that we can expect the following results from the project: the construction of a common vocabulary for tightening the collaboration between the two scientific domains and creating new research topics. By creating this context, we expect to attract (and even train) more trans-disciplinary researchers.

At the boundaries of the MANAO project lie issues in human and machine vision. We have to deal with the former whenever a human observer is taken into account. On one side, computational models of human vision are likely to guide the design of our algorithms. On the other side, the study of interactions between light, shape, and matter may shed some light on the understanding of visual perception. The same kind of connections are expected with machine vision. On the one hand, traditional computational methods for
acquisition (such as photogrammetry) are going to be part of our toolbox. On the other hand, new display technologies (such as the ones used for augmented reality) are likely to benefit from our integrated approach and systems. In the MANAO project we are mostly users of results from human vision. When required, some experimentation might be done in collaboration with experts from this domain, like with the European PRISM project. For machine vision, provided the tight collaboration between optical and digital systems, research will be carried out inside the MANAO project.

Analysis and modeling rely on tools from applied mathematics such as differential and projective geometry, multi-scale models, frequency analysis [45] or differential analysis [77], linear and non-linear approximation techniques, stochastic and deterministic integrations, and linear algebra. We not only rely on classical tools, but also investigate and adapt recent techniques (e.g., improvements in approximation techniques), focusing on their ability to run on modern hardware: the development of our own tools (such as Eigen) is essential to control their performances and their abilities to be integrated into real-time solutions or into new instruments.

3.2. Research axes

The MANAO project is organized around four research axes that cover the large range of expertise of its members and associated members. We briefly introduce these four axes in this section. More details and their inter-influences that are illustrated in the Figure 2 will be given in the following sections.

Axis 1 is the theoretical foundation of the project. Its main goal is to increase the understanding of light, shape, and matter interactions by combining expertise from different domains: optics and human/machine vision for the analysis and computer graphics for the simulation aspect. The goal of our analyses is to identify the different layers/phenomena that compose the observed signal. In a second step, the development of physical simulations and numerical models of these identified phenomena is a way to validate the pertinence of the proposed decompositions.

In Axis 2, the final observers are mainly physical captors. Our goal is thus the development of new acquisition and display technologies that combine optical and digital processes in order to reach fast transfers between real and digital worlds, in order to increase the convergence of these two worlds.

Axes 3 and 4 focus on two aspects of computer graphics: rendering, visualization and illustration in Axis 3, and editing and modeling (content creation) in Axis 4. In these two axes, the final observers are mainly human users, either generic users or expert ones (e.g., archaeologist [81], computer graphics artists).

3.3. Axis 1: Analysis and Simulation

Challenge: Definition and understanding of phenomena resulting from interactions between light, shape, and matter as seen from an observer point of view.

Results: Theoretical tools and numerical models for analyzing and simulating the observed optical phenomena.

To reach the goals of the MANAO project, we need to increase our understanding of how light, shape, and matter act together in synergy and how the resulting signal is finally observed. For this purpose, we need to identify the different phenomena that may be captured by the targeted observers. This is the main objective of this research axis, and it is achieved by using three approaches: the simulation of interactions between light, shape, and matter, their analysis and the development of new numerical models. This resulting improved knowledge is a foundation for the researches done in the three other axes, and the simulation tools together with the numerical models serve the development of the joint optical/digital systems in Axis 2 and their validation.

One of the main and earliest goals in computer graphics is to faithfully reproduce the real world, focusing mainly on light transport. Compared to researchers in physics, researchers in computer graphics rely on a subset of physical laws (mostly radiative transfer and geometric optics), and their main concern is to efficiently use the limited available computational resources while developing as fast as possible algorithms. For this purpose, a large set of theoretical as well as computational tools has been introduced to take a maximum benefit of hardware specificities. These tools are often dedicated to specific phenomena (e.g., direct or
indirect lighting, color bleeding, shadows, caustics). An efficiency-driven approach needs such a classification of light paths [51] in order to develop tailored strategies [93]. For instance, starting from simple direct lighting, more complex phenomena have been progressively introduced: first diffuse indirect illumination [49], [85], then more generic inter-reflections [58], [43] and volumetric scattering [82], [40]. Thanks to this search for efficiency and this classification, researchers in computer graphics have developed a now recognized expertise in fast-simulation of light propagation. Based on finite elements (radiosity techniques) or on unbiased Monte Carlo integration schemes (ray-tracing, particle-tracing, ...), the resulting algorithms and their combination are now sufficiently accurate to be used-back in physical simulations. The MANAO project will continue the search for efficient and accurate simulation techniques, but extending it from computer graphics to optics. Thanks to the close collaboration with scientific researchers from optics, new phenomena beyond radiative transfer and geometric optics will be explored.

Search for algorithmic efficiency and accuracy has to be done in parallel with numerical models. The goal of visual fidelity (generalized to accuracy from an observer point of view in the project) combined with the goal of efficiency leads to the development of alternative representations. For instance, common classical finite-element techniques compute only basis coefficients for each discretization element: the required discretization density would be too large and to computationally expensive to obtain detailed spatial variations and thus visual fidelity. Examples includes texture for decorrelating surface details from surface geometry and high-order wavelets for a multi-scale representation of lighting [39]. The numerical complexity explodes when considering directional properties of light transport such as radiance intensity (Watt per square meter and per steradian - \(W.m^{-2}.sr^{-1}\)), reducing the possibility to simulate or accurately represent some optical phenomena. For instance, Haar wavelets have been extended to the spherical domain [84] but are difficult to extend to non-piecewise-constant data [87]. More recently, researches prefer the use of Spherical Radial Basis Functions [90] or Spherical Harmonics [76]. For more complex data, such as reflective properties (e.g., BRDF [70], [59] - 4D), ray-space (e.g., Light-Field [67] - 4D), spatially varying reflective properties (6D [80]), new models, and representations are still investigated such as rational functions [73] or dedicated models [28] and parameterizations [83], [88]. For each (newly) defined phenomena, we thus explore the space of possible numerical representations to determine the most suited one for a given application, like we have done for BRDF [73].

![Figure 4. First-order analysis [94] have shown that shading variations are caused by depth variations (first-order gradient field) and by normal variations (second-order fields). These fields are visualized using hue and saturation to indicate direction and magnitude of the flow respectively.](image)

Before being able to simulate or to represent the different observed phenomena, we need to define and describe them. To understand the difference between an observed phenomenon and the classical light, shape, and matter decomposition, we can take the example of a highlight. Its observed shape (by a human user or a sensor) is the resulting process of the interaction of these three components, and can be simulated this way. However, this does not provide any intuitive understanding of their relative influence on the final shape:
an artist will directly describe the resulting shape, and not each of the three properties. We thus want to decompose the observed signal into models for each scale that can be easily understandable, representable, and manipulable. For this purpose, we will rely on the analysis of the resulting interaction of light, shape, and matter as observed by a human or a physical sensor. We first consider this analysis from an optical point of view, trying to identify the different phenomena and their scale according to their mathematical properties (e.g., differential [77] and frequency analysis [45]). Such an approach has led us to exhibit the influence of surfaces flows (depth and normal gradients) into lighting pattern deformation (see Figure 4). For a human observer, this corresponds to one recent trend in computer graphics that takes into account the human visual systems [46] both to evaluate the results and to guide the simulations.

3.4. Axis 2: From Acquisition to Display

**Challenge:** Convergence of optical and digital systems to blend real and virtual worlds.

**Results:** Instruments to acquire real world, to display virtual world, and to make both of them interact.

In this axis, we investigate *unified acquisition and display systems*, that is systems which combine optical instruments with digital processing. From digital to real, we investigate new display approaches [67], [54]. We consider projecting systems and surfaces [35], for personal use, virtual reality and augmented reality [30]. From the real world to the digital world, we favor direct measurements of parameters for models and representations, using (new) optical systems unless digitization is required [48], [47]. These resulting systems have to acquire the different phenomena described in Axis 1 and to display them, in an efficient manner [52], [29], [53], [56]. By efficient, we mean that we want to shorten the path between the real world and the virtual world by increasing the data bandwidth between the real (analog) and the virtual (digital) worlds, and by reducing the latency for real-time interactions (we have to prevent unnecessary conversions, and to reduce processing time). To reach this goal, the systems have to be designed as a whole, not by a simple concatenation of optical systems and digital processes, nor by considering each component independently [57].

To increase data bandwidth, one solution is to **parallelize more and more the physical systems**. One possible solution is to multiply the number of simultaneous acquisitions (e.g., simultaneous images from multiple viewpoints [56], [75]). Similarly, increasing the number of viewpoints is a way toward the creation of full 3D displays [67]. However, full acquisition or display of 3D real environments theoretically requires a continuous field of viewpoints, leading to huge data size. Despite the current belief that the increase of computational power will fill the missing gap, when it comes to visual or physical realism, if you double the processing power, people may want four times more accuracy, thus increasing data size as well. To reach the best performances, a trade-off has to be found between the amount of data required to represent accurately the reality and the amount of required processing. This trade-off may be achieved using compressive sensing. Compressive sensing is a new trend issued from the applied mathematics community that provides tools to accurately reconstruct a signal from a small set of measurements assuming that it is sparse in a transform domain (e.g., [74], [99]).
We prefer to achieve this goal by avoiding as much as possible the classical approach where acquisition is followed by a fitting step: this requires in general a large amount of measurements and the fitting itself may consume consequently too much memory and preprocessing time. By preventing unnecessary conversion through fitting techniques, such an approach increase the speed and reduce the data transfer for acquisition but also for display. One of the best recent examples is the work of Cossairt et al. [38]. The whole system is designed around a unique representation of the energy-field issued from (or leaving) a 3D object, either virtual or real: the Light-Field. A Light-Field encodes the light emitted in any direction from any position on an object. It is acquired thanks to a lens-array that leads to the capture of, and projection from, multiple simultaneous viewpoints. A unique representation is used for all the steps of this system. Lens-arrays, parallax barriers, and coded-aperture [64] are one of the key technologies to develop such acquisition (e.g., Light-Field camera [57] and acquisition of light-sources [48]), projection systems (e.g., auto-stereoscopic displays). Such an approach is versatile and may be applied to improve classical optical instruments [62]. More generally, by designing unified optical and digital systems [71], it is possible to leverage the requirement of processing power, the memory footprint, and the cost of optical instruments.

Those are only some examples of what we investigate. We also consider the following approaches to develop new unified systems. First, similar to (and based on) the analysis goal of Axis 1, we have to take into account as much as possible the characteristics of the measurement setup. For instance, when fitting cannot be avoided, integrating them may improve both the processing efficiency and accuracy [73]. Second, we have to integrate signals from multiple sensors (such as GPS, accelerometer, ...) to prevent some computation (e.g., [65]). Finally, the experience of the group in surface modeling help the design of optical surfaces [60] for light sources or head-mounted displays.

3.5. Axis 3: Rendering, Visualization and Illustration

**Challenge:** How to offer the most legible signal to the final observer in real-time?

**Results:** High-level shading primitives, expressive rendering techniques for object depiction, real-time realistic rendering algorithms

![Realistic Rendering Visualization and Illustration](image)

(a) Global illumination [72] (b) Shadows [100] (c) Shape enhancement [96] (d) Shape depiction [27]

*Figure 6. In the MANAO project, we are investigating rendering techniques from realistic solutions (e.g., inter-reflections (a) and shadows (b)) to more expressive ones (shape enhancement (c) with realistic style and shape depiction (d) with stylized style) for visualization.*

The main goal of this axis is to offer to the final observer, in this case mostly a human user, the most legible signal in real-time. Thanks to the analysis and to the decomposition in different phenomena resulting from interactions between light, shape, and matter (Axis 1), and their perception, we can use them to convey essential information in the most pertinent way. Here, the word pertinent can take various forms depending on the application.

In the context of scientific illustration and visualization, we are primarily interested in tools to convey shape or material characteristics of objects in animated 3D scenes. **Expressive rendering** techniques (see Figure 6c,d) provide means for users to depict such features with their own style. To introduce our approach, we detail it from a shape-depiction point of view, domain where we have acquired a recognized expertise. Prior work in this area mostly focused on stylization primitives to achieve line-based rendering [97], [61] or stylized shading [33], [96] with various levels of abstraction. A clear representation of important 3D object features remains a major challenge for better shape depiction, stylization and abstraction purposes. Most existing representations provide only local properties (e.g., curvature), and thus lack characterization of broader shape features. To overcome this limitation, we are developing higher level descriptions of shape [26] with increased robustness to sparsity, noise, and outliers. This is achieved in close collaboration with Axis 1 by the use of higher-order local fitting methods, multi-scale analysis, and global regularization techniques. In order not to neglect the observer and the material characteristics of the objects, we couple this approach with an analysis of the appearance model. To our knowledge, this is an approach which has not been considered yet. This research direction is at the heart of the MANAO project, and has a strong connection with the analysis we plan to conduct in Axis 1. Material characteristics are always considered at the light ray level, but an understanding of higher-level primitives (like the shape of highlights and their motion) would help us to produce more legible renderings and permit novel stylizations; for instance, there is no method that is today able to create stylized renderings that follow the motion of highlights or shadows. We also believe such tools also play a fundamental role for geometry processing purposes (such as shape matching, reassembly, simplification), as well as for editing purposes as discussed in Axis 4.

In the context of real-time photo-realistic rendering (see Figure 6a,b), the challenge is to compute the most plausible images with minimal effort. During the last decade, a lot of work has been devoted to design approximate but real-time rendering algorithms of complex lighting phenomena such as soft-shadows [98], motion blur [45], depth of field [86], reflexions, refractions, and inter-reflexions. For most of these effects it becomes harder to discover fundamentally new and faster methods. On the other hand, we believe that significant speedup can still be achieved through more clever use of massively parallel architectures of the current and upcoming hardware, and/or through more clever tuning of the current algorithms. In particular, regarding the second aspect, we remark that most of the proposed algorithms depend on several parameters which can be used to trade the speed over the quality. Significant speed-up could thus be achieved by identifying effects that would be masked or facilitated and thus devote appropriate computational resources to the rendering [63], [44]. Indeed, the algorithm parameters controlling the quality vs speed are numerous without a direct mapping between their values and their effect. Moreover, their ideal values vary over space and time, and to be effective such an auto-tuning mechanism has to be extremely fast such that its cost is largely compensated by its gain. We believe that our various work on the analysis of the appearance such as in Axis 1 could be beneficial for such purpose too.

Realistic and real-time rendering is closely related to Axis 2: real-time rendering is a requirement to close the loop between real world and digital world. We have to thus develop algorithms and rendering primitives that allow the integration of the acquired data into real-time techniques. We have also to take care of that these real-time techniques have to work with new display systems. For instance, stereo, and more generally multi-view displays are based on the multiplication of simultaneous images. Brute force solutions consist in independent rendering pipeline for each viewpoint. A more energy-efficient solution would take advantages of the computation parts that may be factorized. Another example is the rendering techniques based on image processing, such as our work on augmented reality [37]. Independent image processing for each viewpoint may disturb the feeling of depth by introducing inconsistent information in each images. Finally, more dedicated displays [54] would require new rendering pipelines.

### 3.6. Axis 4: Editing and Modeling

**Challenge:** Editing and modeling appearance using drawing- or sculpting-like tools through high level representations.

**Results:** High-level primitives and hybrid representations for appearance and shape.
During the last decade, the domain of computer graphics has exhibited tremendous improvements in image quality, both for 2D applications and 3D engines. This is mainly due to the availability of an ever increasing amount of shape details, and sophisticated appearance effects including complex lighting environments. Unfortunately, with such a growth in visual richness, even so-called vectorial representations (e.g., subdivision surfaces, Bézier curves, gradient meshes, etc.) become very dense and unmanageable for the end user who has to deal with a huge mass of control points, color labels, and other parameters. This is becoming a major challenge, with a necessity for novel representations. This Axis is thus complementary of Axis 3: the focus is the development of primitives that are easy to use for modeling and editing.

More specifically, we plan to investigate vectorial representations that would be amenable to the production of rich shapes with a minimal set of primitives and/or parameters. To this end we plan to build upon our insights on dynamic local reconstruction techniques and implicit surfaces [4] [32]. When working in 3D, an interesting approach to produce detailed shapes is by means of procedural geometry generation. For instance, many natural phenomena like waves or clouds may be modeled using a combination of procedural functions. Turning such functions into triangle meshes (main rendering primitives of GPUs) is a tedious process that appears not to be necessary with an adapted vectorial shape representation where one could directly turn procedural functions into implicit geometric primitives. Since we want to prevent unnecessary conversions in the whole pipeline (here, between modeling and rendering steps), we will also consider hybrid representations mixing meshes and implicit representations. Such research has thus to be conducted while considering the associated editing tools as well as performance issues. It is indeed important to keep real-time performance (cf. Axis 2) throughout the interaction loop, from user inputs to display, via editing and rendering operations. Finally, it would be interesting to add semantic information into 2D or 3D geometric representations. Semantic geometry appears to be particularly useful for many applications such as the design of more efficient manipulation and animation tools, for automatic simplification and abstraction, or even for automatic indexing and searching. This constitutes a complementary but longer term research direction.

In the MANAO project, we want to investigate representations beyond the classical light, shape, and matter decomposition. We thus want to directly control the appearance of objects both in 2D and 3D applications (e.g., [91]): this is a core topic of computer graphics. When working with 2D vector graphics, digital artists must carefully set up color gradients and textures: examples range from the creation of 2D logos to the photo-realistic imitation of object materials. Classic vector primitives quickly become impractical for creating illusions of complex materials and illuminations, and as a result an increasing amount of time and skill is required. This is only for still images. For animations, vector graphics are only used to create legible appearances composed of simple lines and color gradients. There is thus a need for more complex primitives that are able to accommodate complex reflection or texture patterns, while keeping the ease of use of vector graphics. For instance, instead of drawing color gradients directly, it is more advantageous to draw flow lines that represent local surface concavities and convexities. Going through such an intermediate structure then allows to deform simple material gradients and textures in a coherent way (see Figure 7), and animate them all at once. The manipulation of 3D object materials also raises important issues. Most existing material models are tailored to faithfully reproduce physical behaviors, not to be easily controllable by artists. Therefore artists learn to tweak model parameters to satisfy the needs of a particular shading appearance, which can quickly become cumbersome as the complexity of a 3D scene increases. We believe that an alternative approach is required, whereby material appearance of an object in a typical lighting environment is directly input (e.g., painted or drawn), and adapted to match a plausible material behavior. This way, artists will be able to create their own appearance (e.g., by using our shading primitives [91]), and replicate it to novel illumination environments and 3D models. For this purpose, we will rely on the decompositions and tools issued from Axis 1.

4. Application Domains

4.1. Physical Systems
Figure 7. Based on our analysis [94] (Axis 1), we have designed a system that mimics texture (left) and shading (right) effects using image processing alone. It takes depth (a) and normal (d) images as input, and uses them to deform images (b-e) in ways that closely approximate surface flows (c-f). It provides a convincing, yet artistically controllable illusion of 3D shape conveyed through texture or shading cues.

Given our close relationships with researchers in optics, one novelty of our approach is to extend the range of possible observers to physical sensors in order to work on domains such as simulation, mixed reality, and testing. Capturing, processing, and visualizing complex data is now more and more accessible to everyone, leading to the possible convergence of real and virtual worlds through visual signals. This signal is traditionally captured by cameras. It is now possible to augment them by projecting (e.g., the infrared laser of Microsoft Kinect) and capturing (e.g., GPS localization) other signals that are outside the visible range. This supplemental information replaces values traditionally extracted from standard images and thus lowers down requirements in computational power. Since the captured images are the result of the interactions between light, shape, and matter, the approaches and the improved knowledge from MANAO help in designing interactive acquisition and rendering technologies that are required to merge the real and the virtual worlds. With the resulting unified systems (optical and digital), transfer of pertinent information is favored and inefficient conversion is likely avoided, leading to new uses in interactive computer graphics applications, like augmented reality, displays and computational photography.

4.2. Interactive Visualization and Modeling

This direction includes domains such as scientific illustration and visualization, artistic or plausible rendering, and 3D modeling. In all these cases, the observer, a human, takes part in the process, justifying once more our focus on real-time methods. When targeting average users, characteristics as well as limitations of the human visual system should be taken into account: in particular, it is known that some configurations of light, shape, and matter have masking and facilitation effects on visual perception. For specialized applications (such as archeology), the expertise of the final user and the constraints for 3D user interfaces lead to new uses and dedicated solutions for models and algorithms.

5. Highlights of the Year

5.1. Highlights of the Year

We are regularly publishing our work at the prestigious conference Siggraph. This year was particularly successful with three plain papers [11], [12], [14].

6. New Software and Platforms

6.1. Eigen

KEYWORD: Linear algebra
**FUNCTIONAL DESCRIPTION:** Eigen is an efficient and versatile C++ mathematical template library for linear algebra and related algorithms. In particular it provides fixed and dynamic size matrices and vectors, matrix decompositions (LU, LLT, LDLT, QR, eigenvalues, etc.), sparse matrices with iterative and direct solvers, some basic geometry features (transformations, quaternions, axis-angles, Euler angles, hyperplanes, lines, etc.), some non-linear solvers, automatic differentiations, etc. Thanks to expression templates, Eigen provides a very powerful and easy to use API. Explicit vectorization is performed for the SSE, Altivec and ARM NEON instruction sets, with graceful fallback to non-vectorized code. Expression templates allow to perform global expression optimizations, and to remove unnecessary temporary objects.

**RELEASE FUNCTIONAL DESCRIPTION:** In 2017, we released three revisions of the 3.3 branch with few fixes of compilation and performance regressions, some doxygen documentation improvements, and the addition of transpose, adjoint, conjugate methods to SelfAdjointView to ease writing generic code.

- Participant: Gaël Guennebaud
- Contact: Gaël Guennebaud
- URL: http://eigen.tuxfamily.org/

### 6.2. Elasticity Skinning

**KEYWORD:** 3D animation

**FUNCTIONAL DESCRIPTION:** Geometric skinning techniques are very popular in the industry for their high performances, but fail to mimic realistic deformations. With elastic implicit skinning the skin stretches automatically (without skinning weights) and the vertices distribution is more pleasing. Our approach is more robust, for instance the angle’s range of joints is larger than implicit skinning.

This software has been ported as a plugin for the Modo software (The Foundry) in collaboration with Toulouse Tech Transfer. This plugin has been bought by The Foundry, which maintains and sells it.

- Participants: Brian Wyvill, Damien Rohmer, Florian Canezin, Gaël Guennebaud, Loïc Barthe, Marie-Paule Cani, Mathias Paulin, Olivier Gourmel and Rodolphe Vaillant
- Partners: Université de Bordeaux - CNRS - INP Bordeaux - Université de Toulouse - Institut Polytechnique de Grenoble - Ecole Supérieure de Chimie Physique Electronique de Lyon
- Contact: Gaël Guennebaud

### 7. New Results

#### 7.1. Analysis and Simulation

**7.1.1. A Two-Scale Microfacet Reflectance Model Combining Reflection and Diffraction**, ,

Adequate reflectance models are essential for the production of photorealistic images. Microfacet reflectance models predict the appearance of a material at the macroscopic level based on microscopic surface details. They provide a good match with measured reflectance in some cases, but not always. This discrepancy between the behavior predicted by microfacet models and the observed behavior has puzzled researchers for a long time. In these papers [14], [24], [19], we show that diffraction effects in the micro-geometry provide a plausible explanation. We describe a two-scale reflectance model (cf. Figure 8), separating between geometry details much larger than wavelength and those of size comparable to wavelength. The former model results in the standard Cook-Torrance model. The latter model is responsible for diffraction effects. Diffraction effects at the smaller scale are convolved by the micro-geometry normal distribution. The resulting two-scale model provides a very good approximation to measured reflectances.
Figure 8. Material reflectance properties are caused by small variations in surface geometry. We separate these surface variations into micro-geometry, of size larger than the wavelength of visible light, and nano-geometry, of size comparable to the wavelength. The latter produces diffraction effects, with wavelength-dependent effects. The former corresponds to the classical Cook-Torrance lobe. We explain how these two levels interact and show that combined together, they reproduce measured materials faithfully, including subtle color shifts.

7.1.2. A Practical Extension to Microfacet Theory for the Modeling of Varying Iridescence

Thin film iridescence permits to reproduce the appearance of leather. However, this theory requires spectral rendering engines (such as Maxwell Render) to correctly integrate the change of appearance with respect to viewpoint (known as goniochromatism). This is due to aliasing in the spectral domain as real-time renderers only work with three components (RGB) for the entire range of visible light. In this work [11], we show how to anti-alias a thin-film model, how to incorporate it in microfacet theory, and how to integrate it in a real-time rendering engine. This widens the range of reproducible appearances with microfacet models (cf. Figure 9).

7.2. From Acquisition to Display

7.2.1. Diffraction effects detection for HDR image-based measurements

Modern imaging techniques have proved to be very efficient to recover a scene with high dynamic range (HDR) values. However, this high dynamic range can introduce star-burst patterns around highlights arising from the diffraction of the camera aperture. The spatial extent of this effect can be very wide and alters pixels values, which, in a measurement context, are not reliable anymore. To address this problem, we introduce [21], [15] a novel algorithm that, utilizing a closed-form PSF, predicts where the diffraction will affect the pixels of an HDR image, making it possible to discard them from the measurement. Our approach gives better results (cf. Figure 10) than common deconvolution techniques and the uncertainty values (convolution kernel and noise) of the algorithm output are recovered.

7.2.2. A low-cost multitouch spherical display: hardware and software design

Spherical multitouch displays offer exciting possibilities but are still costly. In this work [17], we first describe hardware and software considerations to build a more affordable one, with off-the-shelf optical components and 3D printed elements. We exploit the technology of laser-beam steering projectors and use optical tracking for multitouch. Besides, although spherical displays become more and more pervasive, the design of interactive content for these displays still remains difficult as it requires most developers to get familiar with specific tools for managing the output and input. We thus present [18] a framework for developing applications for multitouch spherical displays that makes it possible to create interactive content by programming standard GUI applications, as for example interactive web pages. The principal idea is to adapt the window output
Figure 9. Material appearance such as that of leather is usually reproduced with microfacet models in computer graphics. A more realistic result is achieved by adding a thin-film coating that produces iridescent colors. We replace the classic Fresnel reflectance term with a new Airy reflectance term that accounts for iridescence due to thin-film interference. Our main contribution consists in an analytical integration of the high-frequency spectral oscillations exhibited by Airy reflectance, which is essential for practical rendering in RGB. When the scene is rotated, goniochromatic effects such as subtle purple colors may be observed at grazing angles.

and interaction input of classical GUIs outside the application. To this end, our framework consists of two standalone applications where the first one captures the window output and changes the projection via GPU shaders, and the second one adapts the input with a Node.js server and sends interaction and mouse events. In this way, the same application runs on a standard desktop, and on the spherical display. Advantages of our approach include fast prototyping, and the fact that masses of developers can create applications for spherical displays just as if it were, for example, classical web applications. We believe that our framework will contribute to making spherical displays even more pervasive in the future.

7.3. Rendering, Visualization and Illustration

7.3.1. Example-Based Expressive Animation of 2D Rigid Bodies

We have presented [12] a novel approach to facilitate the creation of stylized 2D rigid body animations. Our approach can handle multiple rigid objects following complex physically-simulated trajectories with collisions, while retaining a unique artistic style directly specified by the user. Starting with an existing target animation (e.g., produced by a physical simulation engine) an artist interactively draws over a sparse set of frames, and the desired appearance and motion stylization is automatically propagated to the rest of the sequence (fig. 11). The stylization process may also be performed in an off-line batch process from a small set of drawn sequences. To achieve these goals, we combine parametric deformation synthesis that generalizes and reuses hand-drawn exemplars, with non-parametric techniques that enhance the hand-drawn appearance of the synthesized sequence. We demonstrate the potential of our method on various complex rigid body animations which are created with an expressive hand-drawn look using notably less manual interventions as compared to traditional techniques.

7.3.2. Edge- and Substrate-based Effects for Watercolor Stylization

We investigated [20] characteristic edge-and substrate-based effects for watercolor stylization. These two fundamental elements of painted art play a significant role in traditional watercolors and highly influence the pigment’s behavior and application. Yet a detailed consideration of these specific elements for the stylization of
Figure 10. Results of the algorithm applied on real HDR images for various camera configurations, with input parameters $D_b = 10$ and $\rho = 5\%$. The wavelengths used for each color channel are $[\lambda_R, \lambda_G, \lambda_B] = [600\,\text{nm}, 540\,\text{nm}, 470\,\text{nm}]$. The segmentation images show the discarded pixels (red), the valid pixels (green), and the under-exposed ones (black). If the HDR images exhibits obvious star shaped patterns, the algorithm detects it, and they are finally removed. Such result is qualitative in nature, because there is no reference HDR image without diffraction. False predictions are present in the first two cases (l), where the diffraction prediction seems rotated from the real one. This problem emerges from the misfit of the lens diaphragm, as discussed in subsection 7.7.1.

Figure 11. Given a set of frames $F^S$ coming from reference 2D rigid body source animations, corresponding hand-animated exemplars $E$, and a new target animation $F^T$, the synthesis algorithm relates physical parameters in $F^S$ and $F^T$ to produce the output stylized sequence $F^O$ that resembles $F^E$.
Figure 12. Our methods allow new and improved edge- and substrate-based effects for watercolor stylization: edge darkening (red), gaps (blue), overlaps (green) and dry-brush (yellow). Still Life, model by Dylan Sisson ©Pixar Animation Studios.

3D scenes has not been attempted before. Through this investigation, we contributed to the field by presenting ways to emulate two novel effects: dry-brush and gaps & overlaps. By doing so, we also found ways to improve upon well-studied watercolor effects such as edge-darkening and substrate granulation. Finally, we integrated controllable external lighting influences over the watercolorized result, together with other previously researched watercolor effects. These effects are combined through a direct stylization pipeline [22] to produce sophisticated watercolor imagery (fig. 12), which retains spatial coherence in object-space and is locally controllable in real-time.

7.3.3. Specular Motion and 3D Shape Estimation

Dynamic visual information facilitates three-dimensional shape recognition. It is still unclear, however, whether the motion information generated by moving specularities across a surface is congruent to that available from optic flow produced by a matte-textured shape. Whereas the latter is directly linked to the first-order properties of the shape and its motion relative to the observer, the specular flow, the image flow generated by a specular object, is less sensitive to the object’s motion and is tightly related to second-order properties of the shape. We therefore hypothesize [13] that the perceived bumpiness (a perceptual attribute related to curvature magnitude) is more stable to changes in the type of motion in specular objects compared with their matte-textured counterparts. Results from two two-interval forced-choice experiments in which observers judged the perceived bumpiness of perturbed spherelike objects support this idea and provide an additional layer of evidence for the capacity of the visual system to exploit image information for shape inference.

7.3.4. The Perception of Hazy Gloss

Most previous work on gloss perception has examined the strength and sharpness of specular reflections in simple bidirectional reflectance distribution functions (BRDFs) having a single specular component. However, BRDFs can be substantially more complex and it is interesting to ask how many additional perceptual dimensions there could be in the visual representation of surface reflectance qualities. To address this, we tested [16] materials with two specular components that elicit an impression of hazy gloss. Stimuli were renderings of irregularly shaped objects under environment illumination, with either a single specular BRDF component, or two such components, with the same total specular reflectance but different sharpness parameters, yielding both sharp and blurry highlights simultaneously. Differently shaped objects were presented side by side
in matching, discrimination, and rating tasks. Our results show that observers mainly attend to the sharpest reflections in matching tasks, but they can indeed discriminate between single-component and two-component specular materials in discrimination and rating tasks. The results reveal an additional perceptual dimension of gloss—beyond strength and sharpness—akin to “haze gloss”. However, neither the physical measurements of Hunter and Harold nor the kurtosis of the specular term predict perception in our tasks. We suggest the visual system may use a decomposition of specular reflections in the perception of hazy gloss, and we compare two possible candidates: a physical representation made of two gloss components, and an alternative representation made of a central gloss component and a surrounding halo component.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. CIFRE PhD contract with Technicolor (2014-2018)

Participants: A. Dufay, X. Granier & R. Pacanowski
For this project, we aim at providing interactive previsualization of complex lighting with a smooth transition to the final solution.


Participants: D. Murray & X. Granier
For this project, we aim at providing expressive rendering techniques for volumes.

8.1.3. CIFRE PhD contract with Imaging Optics (2017-2020)

Participants: C. Herzog & X. Granier
For this project, we aim at developing 3 dimensions X-rays imaging techniques for medical applications.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Carer xD: "Caractérisation et restitution du réel xD"
Currently, the characterization and display of the real world are limited to techniques focusing on a subset of the necessary physical phenomena. A lot of work has been done to acquire geometric properties. However, the acquisition of a geometry on an object with complex reflection property or dynamic behavior is still a challenge. Similarly, the characterization of a material is limited to a uniform object for complex material or a diffuse material when one is interested in its spatial variations.

To reach full interaction between real and virtual worlds (augmented reality, mixed reality), it is necessary to acquire the real world in all its aspects (spatial, spectral, temporal) and to return it as in all these dimensions. To achieve this goal, a number of theoretical and practical tools will be developed around the development of mixed reality solutions and the development of some theoretical framework that supports the entire project.

9.2. National Initiatives

9.2.1. ANR

9.2.1.1. “Young Researcher” VIDA (2017-2021)
LP2N-CNRS-IOGS Inria
Leader R. Pacanowski (LP2N-CNRS-IOGS)
Participant P. Barla (Inria)
9.2.1.2. Context.

Since the beginning of the industrial era, prototyping has been an important stage for manufacturers as a preliminary step before mass production. With the rise of Computer Science and the recent advances of intensive computation, the industry is progressively shifting from a tangible prototype to a fully numerical and virtual prototype with the goal of reducing costs during the R&D phase. During the past few years, the emergence of 3D printers has enabled virtual prototyping methods to take into account, at an early stage, some degree of fabricability, especially regarding the shape of the manufactured object. Beyond the shape of an object, predicting the final appearance of a virtual prototype remains a challenge of high potential for many domains (e.g., furniture, textile, architecture). The challenge is mainly due to the fact that the final appearance of an object is dependent on its shape, the material(s) applied on it as well as the viewing and lighting conditions. As shown in Figure 13, solving the inverse problem that goes from Pictorial Design [A] to the Operational Design [D], where a specialist controls the fabrication process, is very hard and ill-posed.

9.2.1.3. Scientific Objectives.

The VIDA project aims at removing the several scientific locks by establishing a framework for direct and inverse design of material appearance for objects of complex shape. Since the manufacturing processes are always changing and evolving, our goal is to establish a framework that is not tied to a fabrication stage. To provide a rich variety of possible appearances, we will target multi-layered materials. We will ensure that every step of our framework is validated by either predictive simulation and/or measurements of the appearance. To illustrate the fabricability of our results, material samples as well as object samples will be fabricated locally or out-sourced to École des Mines de Saint-Etienne (http://www.mines-stetienne.fr/en/EMSE) or http://www.saint-gobain-recherche.fr Saint-Gobain Recherche and their appearance will also be validated with specific devices developed at the https://www.institutoptique.fr/en Institut d’Optique- http://www.lp2n.fr LP2N.

![Figure 13. The different scales involved in the design of object appearance. (A) Pictorial scale: the object is seen as a whole. (B) Radiometric scale: represents the behaviour of a material when light interacts with it. (C) Microscopic scale: the material is described by physical parameters (e.g., index of refraction, absorption coefficient). (D) Operational scale: the parameters control the machine-dependent fabrication process.]


MANAO
Leader G. Guennebaud
This project aims at the development of novel representations for the efficient rendering and manipulation of highly detailed shapes in a multi-resolution context.

9.2.1.5. ISAR (2014-2018)

POTIOC, MANAO, LIG-CNRS-UJF, Diotasoft
Leader M. Hachet (POTIOC)
The ISAR project focuses on the design, implementation and evaluation of new interaction paradigms for spatial augmented reality, and to systematically explore the design space.

MAVERICK, LP2N-CNRS (MANAO), Musée d’Éthnographie de Bordeaux, OCÉ-Print
Leader N. Holzschuch (MAVERICK)
Local Leader R. Pacanowski (LP2N-CNRS)

Museums are operating under conflicting constraints: they have to preserve the artifacts they are storing, while making them available to the public and to researchers. Cultural artifacts are so fragile that simply exposing them to light degrades them. 3D scanning, combined with virtual reality and 3D printing has been used for the preservation and study of sculptures. The approach is limited: it acquires the geometry and the color, but not complex material properties. Current 3D printers are also limited in the range of colors they can reproduce. Our goal in this project is to address the entire chain of material acquisition and restitution. Our idea is to scan complex cultural artifacts, such as silk cloths, capturing all the geometry of their materials at the microscopic level, then reproduce them for study by public and researchers. Reproduction can be either done through 2.5D printing or virtual reality displays.

9.2.1.7. FOLD-Dyn (2017-2021)

IRIT, IMAGINE, MANAO, TeamTo, Mercenaries
Leader L. Barthe (IRIT)
Local Leader G. Guennebaud (Inria)

The FOLD-Dyn project proposes the study of new theoretical approaches for the effective generation of virtual characters deformations, when they are animated. These deformations are two-folds: character skin deformations (skinning) and garment simulations. We propose to explore the possibilities offered by a novel theoretical way of addressing character deformations: the implicit skinning. This method jointly uses meshes and volumetric scalar functions. By improving the theoretical properties of scalar functions, the study of their joint use with meshes, and the introduction of a new approach and its formalism - called multi-layer 3D scalar functions - we aim at finding effective solutions allowing production studios to easily integrate in their pipeline plausible character deformations together with garment simulations.

9.2.2. Competitivity Clusters

9.2.2.1. LabEx CPU

IMB (UPR 5251), LABRI (UMR 5800), Inria (CENTRE BORDEAUX SUD-OUEST), I2M (NEW UMR FROM 2011), IMS (UMR 5218), CEA/DAM

Some members of MANAO participate in the local initiative CPU. As it includes many thematics, from fluid mechanics computation to structure safety but also management of timetable, safety of networks and protocols, management of energy consumption, etc., numerical technology can impact a whole industrial sector. In order to address problems in the domain of certification or qualification, we want to develop numerical sciences at such a level that it can be used as a certification tool.

9.3. International Research Visitors

9.3.1. Visits of International Scientists

Invited professor: Pierre Poulin, professor at Université de Montréal, Visiting scholar program of IdEx Bordeaux

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Chair of Conference Program Committees

Eurographics 2017 Posters chair
10.1.1.2. Member of the Conference Program Committees


10.1.1.3. Reviewer


10.1.2. Journal

10.1.2.1. Reviewer - Reviewing Activities


10.1.3. Scientific Expertise

Horizon 2020 Program

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

The members of our team are involved in teaching computer science at University of Bordeaux, ENSEIRB Engineering School, and Institut d’Optique Graduate School (IOGS). General computer science is concerned, as well as the following graphics related topics:


Master : Gaël Guennebaud & Antoine Lucat, Numerical Techniques, 45 HETD, M1, IOGS, France

Master : Xavier Granier, Image Synthesis, 14 HETD, M2, IOGS, France

Master : Gaël Guennebaud, Geometric Modeling, 22 HETD, M2, IOGS, France

Master : Gaël Guennebaud, Thibaud Lambert, Parallel Programming, 19 HETD, M1, IOGS, France

Master : Romain Pacanowski, Thibaud Lambert, Antoine Lucat & Brett Ridel, Algorithmic and Object Programming, 60 HETD, M1, IOGS, France

Master : Xavier Granier, Romain Pacanowski, Colorimetry and Appearance Modeling, 20 HETD, M1, IOGS, France.

Master : Gaël Guennebaud and Pierre Bénard, 3D Worlds, 60 HETD, M1, Univ. Bdx and IOGS, France.

Master : Pierre Bénard, Virtual Reality, 24 HETD, M2, Univ. Bdx, France.

Master : Patrick Reuter, Graphical user interfaces and Spatial augmented reality seminars, M2, ESTIA, France.

Master : Pierre Bénard, Image Synthesis and 3D modeling, 20 HETD, M2, ENSEIRB, France.


Some members are also in charge of some fields of study:

Master : Xavier Granier, M2, IOGS (Bordeaux), France.

License : Patrick Reuter, Science and Modeling, L2, Univ. Bdx, France.
10.2.2. Supervision

HdR : Pascal Barla, Toward a Perceptually-relevant Theory of Appearance, Inria & Univ. Bordeaux, 9 October 2017


PhD : Thibaud Lambert, Real-time rendering of highly detailed 3D models, Inria & Univ. Bordeaux, 18 December 2017, G. Guennebaud & P. Bénard

PhD in progress : Loïs Mignard-Debize, Plenoptic function and its application to spatial augmented reality, Inria & Univ. Bordeaux, P. Reuter & I. Ihrke

PhD in progress : Antoine Lucat, Appearance Acquisition and Rendering, IOGS & Univ. Bordeaux, R. Pacanowski & X. Granier

PhD in progress : David Murray, Expressive Rendering of Volumetric Data, Thermo Fisher Scientific & Univ. Bordeaux, J. Baril & X. Granier

PhD in progress : Thomas Crespel, Autostereoscopic 3D display, Inria & Univ. Bordeaux, P. Reuter & X. Granier

PhD in progress : Charlotte Herzog, 3 dimensions X-rays imaging for medical applications, Imaging Optics, IOGS & Univ. Bordeaux, X. Granier


10.3. Popularization

We took part in "FACTS", the art and science festival of Université de Bordeaux, and more precisely in the exhibition "Open Lab", which took place from November 14 to 21 at Espace 29. In collaboration with the artist Maud Mulliez, we presented our ongoing work, "L’empreinte du Geste", which aims at analyzing the connection between the gesture of the artist and the mark that the brush or pen produces on the final art piece. An installation combining videos and projection was allowing the audience to discover our preliminary results.

Pierre Bénard gave a talk titled L’art et la science des films d’animation 3D during the internal Inria BSO seminar "Unithé ou café" in January 2017 (45 minutes + questions) and in front of secondary students (120 split into 5 groups) during "la Fête de la Science" (30 minutes) in September 2017. This talk presents the main steps and ingredients required to create a 3D animated film (3D modeling, animation, lighting, rendering) and, for each of them, it shows the subtle but indispensable mix of physical and mathematical models, computer algorithms and artistic talent that it implies. It also highlights how the work of manao contributes to this field.

11. Bibliography

Major publications by the team in recent years


Publications of the year

Articles in International Peer-Reviewed Journal


**International Conferences with Proceedings**


**Conferences without Proceedings**


**Other Publications**


**References in notes**


Project-Team MEMPIS

Modeling Enablers for Multi-PHysics and InteractionS

IN PARTNERSHIP WITH:
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations
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Project-Team MEMPESIS

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 October 01

Keywords:

Computer Science and Digital Science:
  A6. - Modeling, simulation and control
  A6.1.1. - Continuous Modeling (PDE, ODE)
  A6.1.5. - Multiphysics modeling
  A6.2.1. - Numerical analysis of PDE and ODE
  A6.3.1. - Inverse problems
  A6.3.2. - Data assimilation
  A6.3.4. - Model reduction

Other Research Topics and Application Domains:
  B1.1.9. - Bioinformatics
  B2.2.1. - Cardiovascular and respiratory diseases
  B4.3.2. - Hydro-energy
  B4.3.3. - Wind energy
  B5.2.1. - Road vehicles
  B5.2.3. - Aviation
  B5.2.4. - Aerospace
  B5.5. - Materials
  B8.4. - Security and personal assistance
  B8.4.1. - Crisis management

1. Personnel

Research Scientist
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  Aaf Bouharguane [Univ de Bordeaux, Associate Professor]
  Charles-Henri Bruneau [Univ de Bordeaux, Professor]
  Lisl Weynans [Univ de Bordeaux, Associate Professor, until May 2017]

Technical Staff
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  Matias Hastaran [Inria, from Mar 2017]
  Romain Leguay [Inria, from Jun 2017]

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  Emanuela Abbate [Universita degli Studi dell’Insubria / Univ. de Bordeaux]
  Luis Henrique Benetti Ramos [ONERA, from Sep 2017]
  Mathias Braun [IRSTEIA]
  Meriem Jedouaa [Inria, until Jan 2017]
  Baptiste Lambert [Univ de Bordeaux]
  Claire Morel [VALEOL]
2. Overall Objectives

2.1. Multi-physics numerical modeling

We aim at a step change in multi-physics numerical modeling by developing two fundamental enablers:

- reduced-order models;
- hierarchical Cartesian schemes.

Reduced-order models (ROMs) are simplified mathematical models derived from the full set of PDEs governing the physics of the phenomenon of interest. ROMs can be derived from first principles or be data-driven. With ROMs one trades accuracy for speed and scalability, and counteracts the curse of dimension by significantly reducing the computational complexity. ROMs represent an ideal building block of systems with real-time requirements, like interactive decision support systems that offer the possibility to rapidly explore various alternatives.

Hierarchical Cartesian schemes allow the multi-scale solution of PDEs on non body-fitted meshes with a drastic reduction of the computational setup overhead. These methods are easily parallelizable and they can efficiently be mapped to high-performance computer architectures. They avoid dealing with grid generation, a prohibitive task when the boundaries are moving and the topology is complex and unsteady.

3. Research Program

3.1. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions \[37\], \[31\] and boundary conditions are imposed using appropriate interpolation methods \[22\], \[39\], \[35\]. This eliminates the need for boundary conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.
Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical non-structured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are presently virtually absent at Inria, are among the main scientific challenges of our team.

3.2. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the solution of new problem in physics and the prediction of new phenomena thanks to simulation. However, in industrial applications fast on line responses are needed for design and control. For instance, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known a priori. Therefore the aerodynamic and inertial forces are calculated at a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design will experience in service. A simplistic estimate of the number of analyses required would multiply the numbers of conditions to give $10^7$. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical loads conditions, meaning that approximately $10^5$ simulations are required for conventional aircraft configurations. Furthermore these analyses have to be repeated every time that there is an update in the aircraft structure...

Compared to existing approaches for ROMs [28], our interest will be focused on two axis. On the one hand, we start from the consideration that small, highly non-linear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place close to the walls at the scale of a millimeter for computational domains that are of the order of hundreds of meters. In this context our approach is characterized by a multi-scale model where the large scales are described by far field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered.

However, thanks to Proper Orthogonal Decomposition (POD) [32], [38], [25] we can accurately approximate large solution databases using a small base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [33], [23], Dynamic Mode Decomposition [36]) allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between the modes in parameter space, thanks to ideas relying on optimal transportation [40], [27] that we have started developing in the FP7 project FFAST and H2020 AEROGUST. In the following we precise these ideas on a specific example.

4. Application Domains

4.1. Energy conversion
We consider applications in the domain of wind engineering and sea-wave converters. As an example of application of our methods, we show a recent realization where we model a sea-wave energy converter, see figure 1. In this unsteady example, the full interaction between the rigid floater, air and water is described by a monolithic model, the Newton’s law, where physical parameters such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [37]. The background method for fluid structure interface is the volume penalization method [22] where the level set functions is used to improve the degree of accuracy of the method [26] and also to follow the object. The simulations are unsteady, three dimensional, with $O(10^8)$ grid points on 512 CPUs.

![Figure 1. Numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.](image)

4.2. Impacts

The numerical modelling of multimaterial rapid dynamics in extreme conditions is an important technological problem for industrial and scientific applications. Experiments are dangerous, need heavy infrastructures and hence are difficult and expensive to realize. The simulation of such phenomena is challenging because they couple large deformations and displacements in solids to strongly non-linear behaviour in fluids. In what follows, we privilege a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws. This approach was introduced in [30] and subsequently pursued and extended for example in [34], [29], [24], [41].

We study hyper-velocity phenomena where several materials are involved. An example of this approach is the impact of a projectile immersed in air over a shield, see figure 2. Using the same set of equations across the entire domain, we model the compressible fluid, the hyperelastic material and the interaction at the interface that models possible rebounds. Only the constitutive laws characterize the different materials. The simulation is performed over a $4000^2$ fixed Cartesian grid so that the resulting numerical scheme allows an efficient parallelization (512 processors in this case) with an isomorphism between grid partitioning and processor topology. The challenge for our team is to increase the accuracy of the simulation thanks to grid refinement in the vicinity of the moving interfaces, still guaranteeing scalability and a simple computational set up.

4.3. New materials
Thanks to the multi-scale schemes that we develop, we can characterize new materials from constituents. As an example, consider the material presented in figure 3 left. It is a picture of a dry foam that is used as dielectric material. This micrography is taken at the scale of the dry bubbles, where on the surface of the bubble one can observe the carbon nanotubes as white filaments. The presence of nanotubes in the dry emulsion makes the electrical capacitance of this material significantly affected by its strain state by creating aligned dipoles at a larger scale compared to the size of the dielectric molecules. It is a typical multi-scale phenomenon in presence of widely varying physical properties. This material is used to generate micro currents when it undergoes vibrations. The schemes that we devise allow to model this multi-scale irregular material by a monolithic model (same equation in the whole domain), in this case a variable coefficient diffusion equation. In order to recover adequate accuracy, the numerical scheme is adapted near the interfaces between the different subdomains. The computational hierarchical mesh is directly derived by the micrography of the material (figure 3 right).

Figure 3. A micrography of an electrostrictive material is shown on the left: the bright regions visualize the carbon nanotubes. The hierarchical grid adapted to the nanotubes is shown on the right. The ratio between the largest and the smallest cell side is $2^7$. Project developed in collaboration with the CRPP physics and chemistry lab of the CNRS in Bordeaux (Annie Colin, Philippe Poulin).

4.4. Bio-inspired robotic swimming
In bioinspired robotic swimming the aim is of simulating a three-dimensional swimmer starting from pictures. The first step is to build the three-dimensional fish profile based on two-dimensional data retrieved from the picture of an undeformed fish at rest. This is done by a skeleton technique and a three-dimensional level set function describing the body surface. Then the skeleton is deformed using an appropriate swimming law to obtain a sequence of level set functions corresponding to snapshots of the body surface uniformly taken at different instants.

Thanks to skeleton deformation we typically reconstruct 20\% of the snapshots necessary to simulate a swimming stroke, since the time scale of the simulation is significantly smaller than the time step between two subsequent reconstructed snapshots. Also, the surface deformation velocity is required to set the boundary conditions of the flow problem. For this reason it is necessary to build intermediate level set functions and to compute the deformation velocity field between subsequent fish snapshots. Optimal transportation is well suited to achieve this goal providing an objective model to compute intermediate geometries and deformation velocities.

Numerical simulations have been performed in 3D, see figure 4. However, it has been observed that these algorithms do not preserve the physics/features of the represented objects. Indeed, the fish tends to compress during the deformation.

Figure 4. Comparison of the exact deformation velocity (presented inside the swimmer) and the approximated velocity identified using optimal transport (represented outside the fish). The error of the identification scheme is negligible for this component of the velocity, as it can be inferred by comparing the two velocities on the boundary of the swimmer.

For this reason, we will consider incompressible or rigid transports. Another example of bio-inspired swimming is presented in the highlights section.

5. Highlights of the Year

5.1. Highlights of the Year

Memphis team of Inria and VALOREM are both involved in the european project AeroGust (Aeroelastic gust modelling). One of the task aims to investigate the behaviour of wind turbine blades submitted to gust using incompressible flow model and Octree grids. An other task is to carry on an experimental work on a wind turbine. Interests will be first to have real data and use it to better understand the effects of wind and more precisely of gusts, on wind blades. A second interest is to use experimental data to calibrate our numerical schemes in the high-fidelity CFD code.
The measurement of the wind was considered as the most important data to be obtained from the very start of the project. Indeed, this data will be used as a key input for the numerical simulations. This is needed to represent the wind as it arrives at the wind turbine. Then, wind turbine data collection aims to observe the aero-elastic behaviour of wind blades. So, the measurement of blade deformations will allow to check the structural beam model of the blade and to observe its structural behaviour. To observe the aerodynamic load on the wind blade, the measurement of pressure of air on the blade is of significant interest.

A meteorological mast has so been installed in March 2017 in Brittany (France) to measure wind on-site. In figure 5 can be seen a photograph of the whole mast after its installation. Figure 6 contains a picture focused on the sensors of the met mast which are wind vanes for the direction and anemometers for the velocity.

![Figure 5. Photo of the met mast after its installation](image1)

![Figure 6. Photo of the sensors on the met mast](image2)
For the instrumentation of the wind blade, the setup consists of 4 optical fibres along the blade. Each fibre has 4 sensors (pressure or strain gauges) and also temperature sensors at different lengths in order to calibrate the other sensors with respect to temperature. 10 strain gauges and 6 pressure sensors have so been installed on a wind blade located near the meteorological mast (in a way that in the main wind direction, the met mast and the wind turbine are aligned). In figure 7, the 2 lines of sensors going along the pressure side and the leading edge of the wind blade can be seen.

![Figure 7. Photo of the pressure side of the wind blade after instrumentation](image)

Work is now in progress with the experimental data in order to identify different gust conditions in the field and to analyse the effects on the blade deformations. One of the outcomes will be then to compute simulations with our high-fidelity numerical tool developed with VALOREM. This comparison will allow us to calibrate the numerical schemes thanks to real test data.

6. New Software and Platforms

6.1. COCOFLOW

**Keywords:** 3D - Elasticity - MPI - Compressible multimaterial flows  
**Functional Description:** The code is written in fortran 95 with a MPI parallelization. It solves equations of conservation modeling 3D compressible flows with elastic models as equation of state.

- Contact: Florian Bernard  
- URL: https://gforge.inria.fr/projects/cocoflow

6.2. KOPPA

*Kinetic Octree Parallel PolyAtomic*
**FUNCTIONAL DESCRIPTION:** KOPPA is a C++/MPI numerical code solving a large range of rarefied flows from external to internal flows in 1D, 2D or 3D. Different kind of geometries can be treated such as moving geometries coming from CAO files or analytical geometries. The models can be solved on Octree grids with dynamic refinement.

- Participant: Florian Bernard
- Contact: Florian Bernard
- URL: [https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary](https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary)

### 6.3. NaSCar

*Navier-Stokes Cartesian*

**KEYWORDS:** HPC - Numerical analyse - Fluid mechanics - Langage C - PETSc

**SCIENTIFIC DESCRIPTION:** NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

**FUNCTIONAL DESCRIPTION:** This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam’s type. The code is written in C language and use Petsc library for the resolution of large linear systems in parallel.

NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Participant: Michel Bergmann
- Contact: Michel Bergmann
- URL: [https://gforge.inria.fr/projects/nascar/](https://gforge.inria.fr/projects/nascar/)

### 6.4. NS-penal

*Navier-Stokes-penalization*

**KEYWORDS:** 3D - Incompressible flows - 2D

**FUNCTIONAL DESCRIPTION:** The software can be used as a black box with the help of a data file if the obstacle is already proposed. For new geometries the user has to define them. It can be used with several boundary conditions (Dirichlet, Neumann, periodic) and for a wide range of Reynolds numbers.

- Partner: Université de Bordeaux
- Contact: Charles-Henri Bruneau

### 7. New Results

#### 7.1. Fluid-structure interaction and a monolithic scheme

Fluid-structure interaction (FSI) problems are still today difficult to solve on the numerical point of view. Memphis team works on the development of a new numerical method for the simulation of these phenomenas. This method relies on a FSI coupling scheme called "monolithic", in which an eulerian hyperelastic model (Mooney-Rivlin) predicts the behaviour of an elastic structure, all of this in the context of an implicit inclusion of the geometry. A 2D axi-symmetric incompressible Navier-Stokes model is used to follow the behaviour of a newtonian fluid, interacting with this elastic body.
With this coupling method, the solid and fluid problems are solve as a unique numerical solver. This approach has already been studied in the Memphis team for compressible fluids. This process seems to be interesting while it competes on the accuracy point of view with the partitioned approaches, commonly used in the literature. More over, an eulerian formalism releases us from the constraints related to the tracking of the fluid-structure interface, which remains the key difficulty for lagrangian methods. This implicit consideration is therefore coherent from the perspective of including complexe geometries. In responding to difficulties related to the monolithic scheme, we employ a kind of meshing, particularly adapted to AMR (Adaptative Mesh Refinement). Developed by the OPTIMAD society, the library PABLO offers the ability to build conceptually simple meshes, natively parallel, and convenient to use. The hierarchical cartesian meshes are also particularly adapted to complex geometries.

The fluid-structure interface is followed via a level-set function. This one is transported in time with a 2nd order semi-lagrangian scheme which is volume conservative, and it is frequently reinitialize with a redistanciation algorithm. A linear extrapolation algorithm (Aslam) is besides added as a complement to the elastic model in order to limit the "non physical" effects introduced by the monolithic coupling scheme. Finally, a contact model is employed to model the collision between an elastic solid and a rigid solid which can occur in particular in a cardiac pump based on oscillating membranes.

Figure 8. Two FSI problems. On the left: elastic cylinder colliding a rigid plate; on the right: hyperelastic membrane immersed in a pump geometry, moving thanks to a mechanical oscillating actuator.

7.2. A Local Lubrication Model for Spherical Particles within an Incompressible Navier-Stokes Flow

The lubrication effects are short-range hydrodynamic interactions essential to the suspension of the particles, and are usually underestimated by direct numerical simulations of particle laden flows.

A local lubrication correction model for particle laden flow of spherical solid particles has been presented and validated. Interactions between a particle and an obstacle (another particle or a wall) can be decomposed into three types: long range hydrodynamics, short range hydrodynamics also called lubrication effects, and mechanical solid-solid contacts.

Long range hydrodynamic interaction are fully resolved by the Volume Penalization method (VP). The incompressible Navier-Stokes equations have been discretized in time using a scalar projection method and in space with a fully second order penalty method.

Due to unresolved scales associated with the grid, short range hydrodynamic interactions are only partially captured by the numerical approach. We thus introduce a local lubrication model. This correction is based on asymptotic expansions of analytical solutions of particle-particle or particle-wall interactions, assuming that the flow within the gap between the particle and the obstacle is in the Stokes regime. Lubrication forces and torques are corrected in a neighborhood of the contact point of two interacting particles where lubrication is poorly captured, as long as the normalized gap width $\epsilon$ is smaller than a critical length $\epsilon_{\text{lub}}$ (a model parameter).
Finally, a linear soft-sphere collision model is used for solid-solid contacts. This model, widely used in the literature [Costa15, Izard14], represents mechanical contacts as two spring-dashpot systems connected at the contact point. The model allows stretching the collision time, to avoid computational overhead in the calculation of the collision force, making the method particularly efficient.

Our local lubrication correction model have been validated on several benchmarks. First, we considered a single particle falling onto a wall at various approach velocities. The comparison with experimental results [Harada01, Joseph01] enables us to validate the dominant lubrication component resulting from the squeezing of the fluid in the gap. The lubrication force and the torque created by the shearing of the fluid in the gap have been validated on oblique particle-wall collisions in dry and wet systems proposed by Joseph and Hunt [Joseph04]. Since lubrication corrections are made locally, our lubrication model does not required tabulation and is compatible to non-spherical particles. The model will be tested for polydisperse flow of ellipsoidal particles in future works.

7.3. Incompressible flow schemes on octrees.

The incompressible Navier-Stokes solver was validated in 2D last years thanks to the computation of the order of convergence. This year, a comparison has been done with data from literature. A first test-case was the flow around a 2-D cylinder. On the figure 9 can be seen a comparison between results from the developed solver and data from literature [Ploumhans (2000)].

![Figure 9. Comparison of drag coefficients between the code developed and data from literature for the flow around a cylinder at $Re = 550$](image)

A second test case was the flow around a Naca0012 airfoil. The figure 10 shows the X-Velocity around the airfoil at Re = 1000 with an angle of attack of 15°. A QuadTree grid has been used as can be seen in figure 11. The aerodynamic coefficients have been computed for this test-case and have been compared with data from literature [D. F. Kurtulus (2015)]. With $C_D_{\text{mean}} = 0.3$ and $C_L_{\text{mean}} = 0.6$ the results are in good agreement with $C_D_{\text{mean}} = 0.32$ and $C_L_{\text{mean}} = 0.7$ from literature data gathered in [D. F. Kurtulus (2015)].

Then, a grid adaptation process has been developed. It allows for example to deal with moving bodies and to focus on interesting areas in the computational domain. With user defined criteria, the grid is indeed automatically refined or coarsened. So, this code allows a fast meshing of the computational domain thanks to the penalization approach. An interesting compromise between computational time and accuracy is also reached thanks to the adaptive mesh refinement process. A validation of the adaptive mesh refinement process has been done with a comparison between 2 cases: the case of the flow around a fixed body with an inflow of $1 m.s^{-1}$ and the case of a moving body with a velocity of $1 m.s^{-1}$ in a fixed flow. It can be seen on figure 12.
Figure 10. X-Velocity around a Naca0012 airfoil at $Re = 1000$ with an angle of attack of $15^\circ$

Figure 11. QuadTree grid around a Naca0012 airfoil
An extension of the code to 3-D has been developed and validated. Again, 2 different test-cases has been chosen for the validation. First, the flow around a sphere has been computed at different Reynolds number and a comparison has been done with several data from literature as shown in table 1. The figure 13 shows the X-Velocity of the flow around a sphere at \( Re = 500 \) with Octree grid. A LES turbulence model has been implemented with a Vreman subgrid model. So, the second test-case is the flow around a cylinder at \( Re = 3900 \) with LES. The wake profile at different positions has been compared with experimental data as can be seen in figure 14.

<table>
<thead>
<tr>
<th>( Re )</th>
<th>Present work</th>
<th>[Campregher (2009)]</th>
<th>[Fornberg (1988)]</th>
<th>[Fadlun et al. (2000)]</th>
<th>[Kim et al. (2001)]</th>
<th>[Subramanian (2003)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0.6268</td>
<td>0.675</td>
<td>-</td>
<td>-</td>
<td>0.657</td>
<td>0.653</td>
</tr>
<tr>
<td>500</td>
<td>0.5488</td>
<td>0.52</td>
<td>0.4818</td>
<td>0.476</td>
<td>-</td>
<td>0.555</td>
</tr>
</tbody>
</table>

As the overall aim is to simulate the aeroelastic effects on a wind turbine subjected to gusts, a dynamic beam model with axial, torsional and flexural deformations have been implemented and coupled with the Octree Navier-Stokes solver.

**7.4. Validation of NaSCar at higher Reynolds numbers and Aeroelastic coupling**

A beam finite element model has been implemented in order to study the dynamic behavior of the wind turbine blade. The structural model is linear and can describe bending, torsion and axial deformation. There is the possibility to take into account some coupling effects between bending-torsion and torsion-axial deformation. The implementation of the structural model has been validated by means of different static and dynamic tests. In 15 the Fast Fourier Transform of the tip deflection history is reported; the frequency of the predicted peaks is in good agreement with the theoretical values.

The structural model has been coupled with two different computational fluid dynamics codes: a cartesian code (NASCAR3d) and an octree code (developed by Claire Taymans during her PhD). The coupling requires to compute the loads for the structural model by performing an integral of the fluid forces on a surface mesh.
Figure 13. X-Velocity around a sphere at $Re = 500$

Figure 14. Wake profile at different positions behind a cylinder at $Re = 3900$ obtained by averaging Velocity after a preliminary simulation
The surface mesh is updated at each time step according to the displacement of the structure and this allows to update the level set which is used to impose the effects of the body on the fluid. In order to focus the attention on a single blade of the rotor, the inertial terms (centrifugal and Coriolis forces) have been added in both the fluid solver and in the structural model. This makes it possible to perform a preliminary study of the behavior of a single elastic blade by neglecting the interactions between the different blades and the wind turbine’s tower (see 16).

The turbulent flow around the blade is studied by means of the Vreman Large Eddy Simulation model which has been tested on the flow around a cylinder at Re=3900 and Re=140000. The validation of the model for high reynolds flows required the use of a very fine mesh in order to appropriately simulate turbulent dissipation.

and accurately predict the mean flow field, the results obtained are in good agreement with the experimental data of Cantwell et al\(^0\), as reported in 17.

![Figure 17. Cylinder mean wake velocity profiles, Re=140000](image1)

In order to extend the capability of the code to high Reynolds number a wall function approach has been implemented following the guidelines of De Tullio\(^0\). The main idea of this approach is to impose the value of the velocity in the first fluid cells close to the wall by performing a non-linear interpolation based on wall function which represents the velocity distribution in the turbulent boundary layer (see 18).

![Figure 18. wall correction](image2)

### 7.5. Thoracic implant

We are interested in the simulation of elastic tissue deformation in order to simulate the skin deformation due to the pose of a thoracic implant. These implants are used to fill the sternum cavity of patients affected

---

by Pectus Excavatum syndrom. As a first step, we simulated the skin deformation with a single layer elastic model from the real bones, skin and implant geometries imported from STL files. The implant geometry has been designed on-demand by Anatomik Modeling. The single layer elastic model representing an underskin implant, has been implemented on an octree grid to easily and automatically refine around the different geometries and keep accuracy.

![Figure 19. Left: Automatic refinement around a part of the rib cage. Right: Slice of the signed distance function from rib cage and skin with automatic refinement](image)

The results obtained were qualitatively validated by Anatomik Modeling. The implant actually lays on the rib cage, under the muscles. The next step will be then to include a multi-layer elasticity model to take into account the muscles and other biological soft tissues.

![Figure 20. Left: Skin without implant. Right: Skin simulation with implant under skin](image)

Another problem linked to custom made thoracic implants is the extraction of the so-called surgical plan. It is a critical step necessary to design the implant. This plan corresponds to the surface of the rib cage. To extract it, a mass-spring model has been developed and integrated in a software prototype with a graphical interface. The resulting prototype can be used easily from on any rib cage described by a STL file.

### 8. Bilateral Contracts and Grants with Industry
8.1. Bilateral Contracts with Industry

Ongoing contract with the society VALOREM.

9. Partnerships and Cooperations

9.1. Regional Initiatives

Leading team of the regional project "Investigation and Modeling of Suspensions" with the LOMA and LOF labs in Bordeaux

9.2. National Initiatives

We belong to the GDR AMORE on ROMs.

9.2.1. Starting grants

NEMO (A Numerical Enabler for MultiPhysics Simulations on Octrees) is an action to improve and merge all the main MEMPHIS numerical codes. To achieve this goal we have a 12 months financial support (Inria BSO FRM) for a young engineer. This work will be done with strong interaction the the local Inria BSO SED as well as Philippe Depouilly from the IMB "SED".

SMecH is a start-up project in software edition, carried on by Florian Bernard, research engineer in the MEMPHIS team. The project aims at porting to an industrial level the numerical codes developed by the MEMPHIS team. The different collaboration with industrial partners have highlighted the need of new numerical tools to simulate high complexity phenomena such as atmospheric reentries, multi-material flows or fund-structure interactions, but also to highly automatize the numerical simulation workflow to save engineer time. The research codes developed in the MEMPHIS team could match perfectly to this need thanks to:

- the various innovative multi-physics models implemented
- the use of Hierarchical Cartesian schemes that automatize the treatment of moving geometry with accuracy
- the development of schemes suitable for High Parallel Computing.

This year, the project has been submitted to the DGDT, the Inria department in charge of technological transfert, and has been granted an engineer for 6 months as well as the support of IT-Translation.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

EU research projects were and will be a privileged instrument of diffusion and transfer of our results. The AEROGUST H2020 project involves aeronautical industry (Airbus, Dassault, Piaggio...) and research labs (University of Bristol, DLR, NLR, University of Cape Town) and is dedicated to modeling of aerodynamic gust response for applications. We take part in this project by developing simulation models for unsteady aeroelastic problems and data-driven reduced-order models. We played a similar role for the past in the FP7 project FFAST with the same partners.
9.3.1.1. AEROGUST

Title: Aeroelastic Gust Modelling
Programm: H2020
Duration: May 2015 - April 2018
Coordinator: University of Bristol
Partners:
- Airbus Defence and Space (Germany)
- University of Cape Town (South Africa)
- Dassault Aviation (France)
- Deutsches Zentrum für Luft- und Raumfahrt Ev (Germany)
- Stichting Nationaal Lucht- en Ruimtevaartlaboratorium (Netherlands)
- Numerical Mechanics Applications International (Belgium)
- Optimad Engineering S.R.L. (Italy)
- Piaggio Aero Industries Spa (Italy)
- The University of Liverpool (United Kingdom)
- University of Bristol (United Kingdom)
- Valeol (France)

Inria contact: Angelo IOLLO and Michel Bergmann

Encounters with atmospheric turbulence are a vitally important in the design and certification of many manmade structures such as aircraft and wind turbines. Gusts cause rapid changes in the flow about the structures which leads to rigid and flexible unsteady responses. Knowledge of aircraft/gust interactions is therefore vital for loads estimation during aircraft design as it impacts on control systems and often defines the maximum loads that these structures will experience in service. At present industry typically uses the linear doublet lattice method with static loads corrections from expensive wind tunnel data. The wind tunnel data is created using the final aerodynamic surface in the predicted cruise shape. This means that gust loads come relatively late when the design options have been narrowed. Increased competition and environmental concerns are likely to lead to the adoption of more flexible materials and the consideration of novel configurations, in which case the linear assumptions of the current gust loads process will become unacceptable. To introduce non-linearity into the gust loads process without significantly increasing the cost and time, this project has three main objectives: to carry out investigations using CFD so that the non-linearities in gust interactions are understood; to create a gust loads process that does not require wind tunnel data and hence reduces the need for wind tunnel testing; to develop updated reduced order models for gust prediction that account for non-linearity at an acceptable cost. These investigations will reduce the need for expensive wind tunnel testing and hence lead to time and cost savings at the design stage therefore ensuring that the European aerospace and defense industry remain competitive in the future. The wind turbine industry has similar concerns, with gusts and wind shear restricting the locations available for wind farms. The project will also address these issues using common methodology.

9.3.2. Collaborations with Major European Organizations

Partner 1: Chalmers University (Sweden)

This activity is complemented by several international interactions, in particular with Chalmers University in order to converge towards the real implementation of new control technologies on cars, buses and trucks.

Partner 2: Optimad Engineering, Torino (Italy)
We have a crucial partnership with Optimad Engineering, a spin-off of the Politecnico di Torino. This society has implemented in industrial codes several schemes that we have developed for the past. In exchange, we have access to these codes. One example is Pablo, an octree managing parallel library (http://www.optimad.it/products/pablo/). Three former PhD students at Inria are presently employed in Optimad and several others have spent or will spend a research period in this company in order to get acquainted with code architecture and massive parallelism. This company represents for us an ideal partner for the actual industrial feedback on our methods. As mentioned, we plan to create a local start-up in close collaboration with Optimad. This start-up will respond to actual industrial needs by specific software packages built starting from open source tools that are made available to the applied research community via a consortium. Florian Bernard has been recruited in Memphis for two years with the objective of bringing to a higher maturity level a set of modules developed within the team. He plans to fully invest himself in the creation of the start-up. As for the consortium, we are discussing with several partners including Cineca (Italy HPC center) and Optimad about how to structure such a mutual effort. The Storm Inria team is included in the discussions as a possible partner.

Partner 3: W4E (Wave for Energy) (Italy)
One project is the design of an ISWEC (Inertial See Wave Energy Converter) in collaboration with W4E (Wave for Energy), Optimad and others. The ISWEC is a floater prototype that can extract energy form the sea waves. The mechanism is based on a gyroscope that is rotating due to the passive motion of the floater. This prototype is actually tested in the Mediterranean sea in Italy. We will develop the numerical simulation as well as the shape optimization of the ISWEC.

Partner 4: MRGM (Maladies Rares : Génétique et Métabolisme), Bordeaux University (France)
We develop a collaboration with the MRGM lab. They are interested in the swimming of a zebrafish larvae under genetic modifications. One aim is to quantify the power spent by such fishes to swim after a stimuli reaction. The numerical simulation we develop can help computing integral quantities such as the power. This simulation is challenging due to the coupling several methods like image treatment (from movies given by MRGM), optimal transport and numerical simulations.

Partner 5: CRPP (Centre de recherche Paul Pascal), LOF (Laboratoire du Futur) and LOMA (Laboratoire Ondes et Matière d’Aquitaine) labs, Bordeaux University, France.
We established collaborations with physics and chemistry labs in Bordeaux, namely the CRPP, the LOF and the LOMA. They are concerned with the behavior of many passive (CRPP and LOF) and active (LOMA) particles in an incompressible flow. With these partners, we intend to use a combined experimental and computational approach to calibrate models in the case of dilute and concentrated suspensions. The numerical simulations of such particles can help to understand some underlying phenomena at the particles scale and thus to develop mesoscopic models for the whole system (PhD of Baptiste Lambert, oct. 2015).

9.4. International Research Visitors

9.4.1. Visits to International Teams
We have obtained a grant from the Idex Bordeaux of 10keuro to start a collaboration with Charbel Farhat of Stanford University on ROMs.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Member of the Conference Program Committees
Michel Bergman has co-organized the international conference "Interaction fluide-Structure: Analyse et controle", October 2017 (https://indico.math.cnrs.fr/event/1366/overview)
10.1.2. Journal

10.1.2.1. Member of the Editorial Boards
    Angelo Iollo is in the advisory board of Acta Mechanica.

10.1.2.2. Reviewer - Reviewing Activities
    science, Meccanica.

10.1.3. Invited Talks
    The invited conferences are [10], [8], [13], [14], [9], [11], [15], [7].

10.1.4. Scientific Expertise
    Angelo Iollo is reviewer for national and international programs such as H2020 (EU), ANR (France), PRIN
    (Italy).
    2016-2017: Angelo Iollo is expert for the Italian Ministry of Research: quality evaluation of research products.
    Michel Bergmann: member of the Inria Young Researchers Commission, which allocates PhD and Postdoc
    grants.
    Afaf Bouharguane has participated to the recruitment committee for Associate Professor position in Besancon,
    May 2017
    Angelo Iollo was expert in the Young Investigator Rita Levi Montalcini program, Italy

10.2. Teaching - Supervision - Juries

10.2.1. Teaching
    Four members of the team are Professors or Assistant Professors at Bordeaux University and have a teaching
    duty, which consists in courses and practical exercises in numerical analysis and scientific computing. Michel
    Bergmann (CR) also teaches around 64 hours per year (practical exercises in programation for scientific
    computing).

10.2.2. Supervision
    PhD in progress : Claire Morel, Modélisation aerodynamique 3D d une turbine eolienne, 01/01/2015,
    M., Bergmann M., Iollo A.
    PhD in progress : Federico Tesser, Identification of dense suspensions rheology, 01/11/2014,
    Bergmann M., Iollo A.
    PhD in progress : Baptiste Lambert, modélisation et simulations numériques des contacts dans des
    écoulements chargés en particules, 01/10/2015, Bergmann M., Weynans L.,
    PhD in progress : Emanuela Abbate, Méthodes numériques pour problèmes stiff en mécanique des
    fluides et élasticité, 01/11/2015, Iollo, A.
    PhD in progress : Mathias Braun, Modèles réduits et problèmes inverses pour l étude de la résilience
    des réseaux d eau potable, 01/10/2015, Iollo A. and Mortazavi I.
    PhD in progress : Luis Henrique Benetti Ramo, Aeroelastic instabilities, Bergmann M. and Iollo A.
    PhD in progress : Guillaume Ravel, Simulation numérique et modélisation de la nage du poisson
    zèbre pour l étude de maladies humaines d origine génétique et toxicologique, 01/10/2017, Bouhar-
    guane A. and Babin P. (MRGM)
PhD in progress: Sebastien Riffaud, Reduced Order Models, classification and data geometry, 01/10/2017, Iollo A.


10.2.3. Juries

Michel Bergmann has participated to the PhD defense of Pierre Costini, Centrale Marseille, 19/05/2017
Michel Bergmann has participated to the PhD defense of Lei Cheng, DELF (pays-bas), 15/12/2017
Angelo Iollo has been reviewer of the PhD defense Applicabilité de la réduction de modèles à la conception aérothermique collaborative des systèmes d’air secondaires des turbomachines, Pierre Costini, Ecole Doctorale des Sciences pour l’Ingénieur, Aix-Marseille, May 2017.
Angelo Iollo has participated to the PhD defense of Manon Deville, Modélisation de l’électroporation et de la transfection de gènes à l’échelle du tissu. Aspects théorique et numérique. " Institut de Mathématiques de Bordeaux, université de Bordeaux, novembre 2017.
Angelo Iollo has participated as president to the PhD defense of Agathe Peretti Quantification de l’hétérogénéité tumorale à partir de l’imagerie médicale. Application à la classification de tumeurs rénales. Institut de Mathématiques de Bordeaux, université de Bordeaux, décembre 2017.

10.3. Popularization

Lisl Weynans has co-organized the Journée Filles et Maths, une équation lumineuse, April 2017.
Afaf Bouharguane and Lisl Weynans have co-organized the Journée Emploi Maths de l’Unité de Formation Mathématiques et Interaction, November 2017.

11. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


Invited Conferences


[10] A. IOLLO.Compressible multimaterial numerical models, in "IperPV 2017 - XVII Italian meeting on hyperbolic equations", Pavia, Italy, September 2017, https://hal.inria.fr/hal-01668533.

International Conferences with Proceedings


Conferences without Proceedings


Research Reports


Other Publications


References in notes


Project-Team MNEMOSYNE

Mnemonic Synergy

IN PARTNERSHIP WITH:
CNRS
Institut Polytechnique de Bordeaux
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Computational Neuroscience and Medicine
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Project-Team MNEMOSYNE

Creation of the Team: 2012 February 01, updated into Project-Team: 2014 July 01

Keywords:

**Computer Science and Digital Science:**
- A1.1.12. - Non-conventional architectures
- A1.5. - Complex systems
- A3.1.1. - Modeling, representation
- A3.1.7. - Open data
- A3.2.2. - Knowledge extraction, cleaning
- A3.2.5. - Ontologies
- A3.3. - Data and knowledge analysis
- A3.3.2. - Data mining
- A3.4.1. - Supervised learning
- A3.4.2. - Unsupervised learning
- A3.4.3. - Reinforcement learning
- A3.4.4. - Optimization and learning
- A3.4.6. - Neural networks
- A3.4.8. - Deep learning
- A5.1.1. - Engineering of interactive systems
- A5.1.2. - Evaluation of interactive systems
- A5.2. - Data visualization
- A5.3.3. - Pattern recognition
- A5.4.1. - Object recognition
- A5.4.2. - Activity recognition
- A5.7.1. - Sound
- A5.7.3. - Speech
- A5.7.4. - Analysis
- A5.8. - Natural language processing
- A5.9.1. - Sampling, acquisition
- A5.10.5. - Robot interaction (with the environment, humans, other robots)
- A5.10.7. - Learning
- A5.10.8. - Cognitive robotics and systems
- A5.11.1. - Human activity analysis and recognition
- A7.1. - Algorithms
- A9.2. - Machine learning
- A9.5. - Robotics

**Other Research Topics and Application Domains:**
- B1.2. - Neuroscience and cognitive science
- B1.2.1. - Understanding and simulation of the brain and the nervous system
- B1.2.2. - Cognitive science
- B2.2.6. - Neurodegenerative diseases
1. Personnel

**Research Scientists**
- Frédéric Alexandre [Team leader, Inria, Senior Researcher, HDR]
- Xavier Hinaut [Inria, Researcher]
- Randa Kassab [Inria, Starting Research position, FUI Sumatra]
- Nicolas Rougier [Inria, Researcher, HDR]
- Thierry Viéville [Inria, Senior Researcher (part-time (50%) in the project-team), HDR]

**Faculty Member**
- André Garenne [Univ de Bordeaux, Associate Professor]

**External Collaborators**
- Arthur Leblois [CNRS, from Oct 2017, HDR]
- Adrian Palacios [Univ. Valparaiso]

**PhD Students**
- Ikram Chraibi Kaadoud [Univ. Bordeaux, PhD Student, granted by CIFRE]
- Thalita Firmo Drumond [Inria]
- Bhargav Teja Nallapu [Inria]
- Silvia Pagliarini [Inria, from Nov 2017]
- Anthony Strock [Univ de Bordeaux, from Sep 2017]

**Post-Doctoral Fellow**
- Fabien Benureau [Inria, until Sep 2017]

**Administrative Assistant**
- Chrystel Plumejeau [Inria, Assistant (part time in the team)]

2. Overall Objectives

2.1. Summary

At the frontier between integrative and computational neuroscience, we propose to model the brain as a system of active memories in synergy and in interaction with the internal and external world and to simulate it as a whole and in situation.

In integrative and cognitive neuroscience (cf. § 3.1), on the basis of current knowledge and experimental data, we develop models of the main cerebral structures, taking a specific care of the kind of mnemonic function they implement and of their interface with other cerebral and external structures. Then, in a systemic approach, we build the main behavioral loops involving these cerebral structures, connecting a wide spectrum of actions to various kinds of sensations. We observe at the behavioral level the properties emerging from the interaction between these loops.
We claim that this approach is particularly fruitful for investigating cerebral structures like the basal ganglia and the prefrontal cortex, difficult to comprehend today because of the rich and multimodal information flows they integrate. We expect to cope with the high complexity of such systems, inspired by behavioral and developmental sciences, explaining how behavioral loops gradually incorporate in the system various kinds of information and associated mnemonic representations. As a consequence, the underlying cognitive architecture, emerging from the interplay between these sensations-actions loops, results from a mnemonic synergy.

In computational neuroscience (cf. § 3.2), we concentrate on the efficiency of local mechanisms and on the effectiveness of the distributed computations at the level of the system. We also take care of the analysis of their dynamic properties, at different time scales. These fundamental properties are of high importance to allow the deployment of very large systems and their simulation in a framework of high performance computing. Running simulations at a large scale is particularly interesting to evaluate over a long period a consistent and relatively complete network of cerebral structures in realistic interaction with the external and internal world. We face this problem in the domain of autonomous robotics (cf. § 3.4) and ensure a real autonomy by the design of an artificial physiology and convenient learning protocols.

We are convinced that this original approach also permits to revisit and enrich algorithms and methodologies in machine learning (cf. § 3.3) and in autonomous robotics (cf. § 3.4), in addition to elaborate hypotheses to be tested in neuroscience and medicine, while offering to these latter domains a new ground of experimentation similar to their daily experimental studies.

3. Research Program

3.1. Integrative and Cognitive Neuroscience

The human brain is often considered as the most complex system dedicated to information processing. This multi-scale complexity, described from the metabolic to the network level, is particularly studied in integrative neuroscience, the goal of which is to explain how cognitive functions (ranging from sensorimotor coordination to executive functions) emerge from (are the result of the interaction of) distributed and adaptive computations of processing units, displayed along neural structures and information flows. Indeed, beyond the astounding complexity reported in physiological studies, integrative neuroscience aims at extracting, in simplifying models, regularities at various levels of description. From a mesoscopic point of view, most neuronal structures (and particularly some of primary importance like the cortex, cerebellum, striatum, hippocampus) can be described through a regular organization of information flows and homogenous learning rules, whatever the nature of the processed information. From a macroscopic point of view, the arrangement in space of neuronal structures within the cerebral architecture also obeys a functional logic, the sketch of which is captured in models describing the main information flows in the brain, the corresponding loops built in interaction with the external and internal (bodily and hormonal) world and the developmental steps leading to the acquisition of elementary sensorimotor skills up to the most complex executive functions.

In summary, integrative neuroscience builds, on an overwhelming quantity of data, a simplifying and interpretative grid suggesting homogenous local computations and a structured and logical plan for the development of cognitive functions. They arise from interactions and information exchange between neuronal structures and the external and internal world and also within the network of structures.

This domain is today very active and stimulating because it proposes, of course at the price of simplifications, global views of cerebral functioning and more local hypotheses on the role of subsets of neuronal structures in cognition. In the global approaches, the integration of data from experimental psychology and clinical studies leads to an overview of the brain as a set of interacting memories, each devoted to a specific kind of information processing [46]. It results also in longstanding and very ambitious studies for the design of cognitive architectures aiming at embracing the whole cognition. With the notable exception of works initiated by [43], most of these frameworks (e.g. Soar, ACT-R), though sometimes justified on biological grounds, do not go up to a connectionist neuronal implementation. Furthermore, because of the complexity of the resulting frameworks, they are restricted to simple symbolic interfaces with the internal and external
world and to (relatively) small-sized internal structures. Our main research objective is undoubtly to build such a general purpose cognitive architecture (to model the brain as a whole in a systemic way), using a connectionist implementation and able to cope with a realistic environment.

3.2. Computational Neuroscience

From a general point of view, computational neuroscience can be defined as the development of methods from computer science and applied mathematics, to explore more technically and theoretically the relations between structures and functions in the brain [48], [36]. During the recent years this domain has gained an increasing interest in neuroscience and has become an essential tool for scientific developments in most fields in neuroscience, from the molecule to the system. In this view, all the objectives of our team can be described as possible progresses in computational neuroscience. Accordingly, it can be underlined that the systemic view that we promote can offer original contributions in the sense that, whereas most classical models in computational neuroscience focus on the better understanding of the structure/function relationship for isolated specific structures, we aim at exploring synergies between structures. Consequently, we target interfaces and interplay between heterogenous modes of computing, which is rarely addressed in classical computational neuroscience.

We also insist on another aspect of computational neuroscience which is, in our opinion, at the core of the involvement of computer scientists and mathematicians in the domain and on which we think we could particularly contribute. Indeed, we think that our primary abilities in numerical sciences imply that our developments are characterized above all by the effectiveness of the corresponding computations: We provide biologically inspired architectures with effective computational properties, such as robustness to noise, self-organization, on-line learning. We more generally underline the requirement that our models must also mimick biology through its most general law of homeostasis and self-adaptability in an unknown and changing environment. This means that we propose to numerically experiment such models and thus provide effective methods to falsify them.

Here, computational neuroscience means mimicking original computations made by the neuronal substratum and mastering their corresponding properties: computations are distributed and adaptive; they are performed without an homoculus or any central clock. Numerical schemes developed for distributed dynamical systems and algorithms elaborated for distributed computations are of central interest here [33], [42] and were the basis for several contributions in our group [47], [44], [49]. Ensuring such a rigor in the computations associated to our systemic and large scale approach is of central importance.

Equally important is the choice for the formalism of computation, extensively discussed in the connectionist domain. Spiking neurons are today widely recognized of central interest to study synchronization mechanisms and neuronal coupling at the microscopic level [34]; the associated formalism [39] can be possibly considered for local studies or for relating our results with this important domain in connectionism. Nevertheless, we remain mainly at the mesoscopic level of modeling, the level of the neuronal population, and consequently interested in the formalism developed for dynamic neural fields [31], that demonstrated a richness of behavior [35] adapted to the kind of phenomena we wish to manipulate at this level of description. Our group has a long experience in the study and adaptation of the properties of neural fields [44], [45] and their use for observing the emergence of typical cortical properties [38]. In the envisioned development of more complex architectures and interplay between structures, the exploration of mathematical properties such as stability and boundedness and the observation of emerging phenomena is one important objective. This objective is also associated with that of capitalizing our experience and promoting good practices in our software production. In summary, we think that this systemic approach also brings to computational neuroscience new case studies where heterogenous and adaptive models with various time scales and parameters have to be considered jointly to obtain a mastered substratum of computation. This is particularly critical for large scale deployments.

3.3. Machine Learning

The adaptive properties of the nervous system are certainly among its most fascinating characteristics, with a high impact on our cognitive functions. Accordingly, machine learning is a domain [41] that aims at
giving such characteristics to artificial systems, using a mathematical framework (probabilities, statistics, data analysis, etc.). Some of its most famous algorithms are directly inspired from neuroscience, at different levels. Connectionist learning algorithms implement, in various neuronal architectures, weight update rules, generally derived from the hebbian rule, performing non supervised (e.g. Kohonen self-organizing maps), supervised (e.g. layered perceptrons) or associative (e.g. Hopfield recurrent network) learning. Other algorithms, not necessarily connectionist, perform other kinds of learning, like reinforcement learning. Machine learning is a very mature domain today and all these algorithms have been extensively studied, at both the theoretical and practical levels, with much success. They have also been related to many functions (in the living and artificial domains) like discrimination, categorisation, sensorimotor coordination, planning, etc. and several neuronal structures have been proposed as the substratum for these kinds of learning [37], [30]. Nevertheless, we believe that, as for previous models, machine learning algorithms remain isolated tools, whereas our systemic approach can bring original views on these problems.

At the cognitive level, most of the problems we face do not rely on only one kind of learning and require instead skills that have to be learned in preliminary steps. That is the reason why cognitive architectures are often referred to as systems of memory, communicating and sharing information for problem solving. Instead of the classical view in machine learning of a flat architecture, a more complex network of modules must be considered here, as it is the case in the domain of deep learning. In addition, our systemic approach brings the question of incrementally building such a system, with a clear inspiration from developmental sciences. In this perspective, modules can generate internal signals corresponding to internal goals, predictions, error signals, able to supervise the learning of other modules (possibly endowed with a different learning rule), supposed to become autonomous after an instructing period. A typical example is that of episodic learning (in the hippocampus), storing declarative memory about a collection of past episods and supervising the training of a procedural memory in the cortex.

At the behavioral level, as mentionned above, our systemic approach underlines the fundamental links between the adaptive system and the internal and external world. The internal world includes proprioception and interoception, giving information about the body and its needs for integrity and other fundamental programs. The external world includes physical laws that have to be learned and possibly intelligent agents for more complex interactions. Both involve sensors and actuators that are the interfaces with these worlds and close the loops. Within this rich picture, machine learning generally selects one situation that defines useful sensors and actuators and a corpus with properly segmented data and time, and builds a specific architecture and its corresponding criteria to be satisfied. In our approach however, the first question to be raised is to discover what is the goal, where attention must be focused on and which previous skills must be exploited, with the help of a dynamic architecture and possibly other partners. In this domain, the behavioral and the developmental sciences, observing how and along which stages an agent learns, are of great help to bring some structure to this high dimensional problem.

At the implementation level, this analysis opens many fundamental challenges, hardly considered in machine learning: stability must be preserved despite on-line continuous learning; criteria to be satisfied often refer to behavioral and global measurements but they must be translated to control the local circuit level; in an incremental or developmental approach, how will the development of new functions preserve the integrity and stability of others? In addition, this continous re-arrangement is supposed to involve several kinds of learning, at different time scales (from msec to years in humans) and to interfer with other phenomena like variability and meta-plasticity.

In summary, our main objective in machine learning is to propose on-line learning systems, where several modes of learning have to collaborate and where the protocoles of training are realistic. We promote here a really autonomous learning, where the agent must select by itself internal resources (and build them if not available) to evolve at the best in an unknown world, without the help of any deus-ex-machina to define parameters, build corpus and define training sessions, as it is generally the case in machine learning. To that end, autonomous robotics (cf. § 3.4) is a perfect testbed.

3.4. Autonomous Robotics
Autonomous robots are not only convenient platforms to implement our algorithms; the choice of such platforms is also motivated by theories in cognitive science and neuroscience indicating that cognition emerges from interactions of the body in direct loops with the world (embodiment of cognition [32]). In addition to real robotic platforms, software implementations of autonomous robotic systems including components dedicated to their body and their environment will be also possibly exploited, considering that they are also a tool for studying conditions for a real autonomous learning.

A real autonomy can be obtained only if the robot is able to define its goal by itself, without the specification of any high level and abstract cost function or rewarding state. To ensure such a capability, we propose to endow the robot with an artificial physiology, corresponding to perceive some kind of pain and pleasure. It may consequently discriminate internal and external goals (or situations to be avoided). This will mimick circuits related to fundamental needs (e.g. hunger and thirst) and to the preservation of bodily integrity. An important objective is to show that more abstract planning capabilities can arise from these basic goals.

A real autonomy with an on-line continuous learning as described in § 3.3 will be made possible by the elaboration of protocols of learning, as it is the case, in animal conditioning, for experimental studies where performance on a task can be obtained only after a shaping in increasingly complex tasks. Similarly, developmental sciences can teach us about the ordered elaboration of skills and their association in more complex schemes. An important challenge here is to translate these hints at the level of the cerebral architecture.

As a whole, autonomous robotics permits to assess the consistency of our models in realistic condition of use and offers to our colleagues in behavioral sciences an object of study and comparison, regarding behavioral dynamics emerging from interactions with the environment, also observable at the neuronal level.

In summary, our main contribution in autonomous robotics is to make autonomy possible, by various means corresponding to endow robots with an artificial physiology, to give instructions in a natural and incremental way and to prioritize the synergy between reactive and robust schemes over complex planning structures.

4. Application Domains

4.1. Overview

One of the most original specificity of our team is that it is part of a laboratory in Neuroscience (with a large spectrum of activity from the molecule to the behavior), focused on neurodegenerative diseases and consequently working in tight collaboration with the medical domain. As a consequence, neuroscientists and the medical world are considered as the primary end-users of our researches. Beyond data and signal analysis where our expertise in machine learning may be possibly useful, our interactions are mainly centered on the exploitation of our models. They will be classically regarded as a way to validate biological assumptions and to generate new hypotheses to be investigated in the living. Our macroscopic models and their implementation in autonomous robots will allow an analysis at the behavioral level and will propose a systemic framework, the interpretation of which will meet aetiological analysis in the medical domain and interpretation of intelligent behavior in cognitive neuroscience.

The study of neurodegenerative diseases is targeted because they match the phenomena we model. Particularly, the Parkinson disease results from the death of dopaminergic cells in the basal ganglia, one of the main systems that we are modeling. The Alzheimer disease also results from the loss of neurons, in several cortical and extracortical regions. The variety of these regions, together with large mnesic and cognitive deficits, require a systemic view of the cerebral architecture and associated functions, very consistent with our approach.

Of course, numerical sciences are also impacted by our researches, at several levels. At a global level, we will propose new control architectures aimed at providing a higher degree of autonomy to robots, as well as machine learning algorithms working in more realistic environment. More specifically, our focus on some cognitive functions in closed loop with a real environment will address currently open problems. This is obviously the case for planning and decision making; this is particularly the case for the domain of affective
computing, since motivational characteristics arising from the design of an artificial physiology allow to consider not only cold rational cognition but also hot emotional cognition. The association of both kinds of cognition is undoubtly an innovative way to create more realistic intelligent systems but also to elaborate more natural interfaces between these systems and human users.

At last, we think that our activities in well-founded distributed computations and high performance computing are not just intended to help us design large scale systems. We also think that we are working here at the core of informatics and, accordingly, that we could transfer some fundamental results in this domain.

5. Highlights of the Year

5.1. Highlights of the Year

We published this year an important article [4] gathering 45 co-authors about the ReScience initiative which makes an important contribution that traditional scientific journals cannot offer. It provides a venue for publishing replication work, which traditional journals exclude for lack of novelty. Considering the ever increasing importance of computational methods in all scientific disciplines, we believe that our approach to replication is of interest to a broad audience of researchers.

6. New Software and Platforms

6.1. DANA

_Distributed Asynchronous Numerical and Adaptive computing framework_

**KEYWORD:** Neural networks

**FUNCTIONAL DESCRIPTION:** DANA is a python framework whose computational paradigm is grounded on the notion of a unit that is essentially a set of time dependent values varying under the influence of other units via adaptive weighted connections. The evolutions of a unit’s value are defined by a set of differential equations expressed in standard mathematical notation which greatly ease their definition. The units are organized into groups that form a model. Each unit can be connected to any other unit (including itself) using a weighted connection. The DANA framework offers a set of core objects needed to design and run such models. The modeler only has to define the equations of a unit as well as the equations governing the training of the connections. The simulation is completely transparent to the modeler and is handled by DANA. This allows DANA to be used for a wide range of numerical and distributed models as long as they fit the proposed framework (e.g. cellular automata, reaction-diffusion system, decentralized neural networks, recurrent neural networks, kernel-based image processing, etc.).

- Participant: Nicolas Rougier
- Contact: Nicolas Rougier

6.2. ENAS

_Event Neural Assembly Simulation_

**KEYWORDS:** Neurosciences - Health - Physiology
Scientific Description: As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS integrating tools for spike trains analysis and simulation. These tools are accessible through a friendly Graphical User Interface that avoids any scripting or writing code from the user. Most of them have been implemented to run in parallel to reduce the time and memory consumption. ENAS offers basic visualizations and classical analysis for statistics of spike trains analysis. It also proposes statistical analysis with Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. ENAS also includes specific tools dedicated to the retina: Receptive Field computation and a virtual retina simulator. Finally, ENAS generates synthetic rasters, either from know statistics or from the VIRTUAL RETINA simulator. We expect ENAS to become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to users feedback. Our goal is to progressively enrich ENAS with the latest research results, in order to facilitate transfer of new methods to the community.

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- Participants: Bruno Cessac, Daniela Pamplona, Geoffrey Portelli, Hassan Nasser, Pierre Kornprobst, Rodrigo Cofre Torres, Sélim Kraria, Theodora Karvouniari and Thierry Viéville
- Contact: Bruno Cessac
- URL: https://enas.inria.fr

6.3. Virtual Enaction

Keywords: Neurosciences - Simulation - Health

Functional Description: VirtualEnaction: A Platform for Systemic Neuroscience Simulation. The computational models studied in this project have applications that extend far beyond what is possible to experiment yet in human or non-human primate subjects. Real robotics experimentations are also impaireed by rather heavy technological constraints, for instance, it is not easy to dismantle a given embedded system in the course of emerging ideas. The only versatile environment in which such complex behaviors can be studied both globally and at the level of details of the available modeling is a virtual environment, as in video games. Such a system can be implemented as “brainy-bot” (a programmed player based on our knowledge of the brain architecture) which goal is to survive in a complete manipulable environment.

In order to attain this rather ambitious objective we both (i) deploy an existing open-source video game middleware in order to be able to shape the survival situation to be studied and (ii) revisit the existing models in order to be able to integrate them as an effective brainy-bot. It consists of a platform associated to a scenario that is the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction) and in which it is easy to integrate an artificial agent with sensory inputs (visual, touch and smell), emotional and somatosensory cues (hunger, thirst, fear, ...) and motor outputs (movement, gesture,
..) connected to a "brain" whose architecture will correspond to the major anatomical regions involved in
the issues of learning and action selection (cortex areas detailed here, basal ganglia, hippocampus, and areas
dedicated to sensorimotor processes). The internal game clock can be slowed down enough to be able to run
non trivial brainy-bot implementations. This platform has already being used by two students of the team and
is now a new deliverable of the KEOps project.

- Participants: André Garenne, Frédéric Alexandre, Nicolas Rougier and Thierry Viéville
- Contact: Frédéric Alexandre

7. New Results

7.1. Overview

This year we have explored two main cortico-basal loops of cerebral architecture, the limbic and motor loops,
and their associated memory mechanisms. The limbic loop (cf. § 7.2) concerns the taking into account of the
emotional and motivational aspects by the respondant and operant conditioning and their relations with the
semantic and episodic memories. The motor loop (cf. § 7.3) considers the evolution of sensorimotor learning,
from goal-directed behaviors to habitual behaviors.

We have also worked on the systemic integration of our models (cf. § 7.4), raising the question of the conditions
of autonomous learning and certain global characteristics such as neuromodulation.

Finally, we study the links between our bio-inspired modeling work and Machine Learning (cf. § 7.5),
revisiting this latter domain in the light of the principles highlighted by our models.

7.2. The limbic loop

We explore the limbic loop by studying a series of neural mechanisms that propose how respondant condition-
ing results from interactions between the amygdala, the nucleus accumbens and the limbic pole of the frontal
cortex. In our models, this learning is also fed by exchanges with the hippocampus (episodic memory) [6]
and the sensory cortex (semantic memory). We have also addressed the difficult question of the articulation
between the respondant and operant conditioning in particular in the nucleus accumbens.

Also in connection with this loop, we studied the dynamics of dopamine release in the midbrain, considered
to play an essential role in the coding of the prediction error. This model [12] developed in the framework
of our collaboration with India (cf. § 9.3) proposes to introduce into the classical circuit, new actors (such as
the pedunculopontine tegmental nucleus in the brainstem) and new functions (dissociation of amplitude and
timing of the reward), that we will seek to corroborate in the future.

7.3. The motor loop

The nervous system structures involved in decision making constitute a circuit formed by the basal ganglia,
the cortex, the thalamus and their numerous interconnections. This circuit can be described as a set of loops
operating in parallel and interacting at different points. The decisions and therefore the actions of an individual
emerge from the interactions between these loops and the plasticity of their connections. These emerging
behaviors and arising learning processes are addressed through a closed-loop approach in which the theoretical
model is in constant interaction with the environment of the task. To this end, neural modeling and dedicated
analysis software tools were developed in the laboratory, at the level of the neuronal circuit.

7.4. Systemic integration

Systemic integration promotes the idea of developing large models that associate several cortico-basal loops
and even other cerebral structures and more generally takes into account the influence of the body on this
network [19]. This requires to propose a global picture for the organization and functional association between
all these elements [18] and to analyze its consequences from a representational point of view [1] and also
concerning autonomous learning [7].
It also requires to evaluate the properties of such systems from their interactions with the body and the environment, as we have done this year using the VirtualEnaction platform.

7.5. Machine Learning

In this section, we report on some neuronal adaptive mechanisms, that we develop at the frontier between Machine Learning and Computational Neuroscience. Our goal is to consider and adapt models in Machine Learning for their integration in a bio-inspired framework. We were interested this year in three paradigms of computation.

The first paradigm concerns the manipulation of temporal sequences. In a perspective of better understanding how the brain learns structured sequences we work on a model on syntax acquisition and Human-Robot Interaction using the Reservoir Computing framework (using random recurrent networks) [24], [15], [17] with our collaborators at the University of Hamburg (cf. § 9.3). A syntactic re-analysis system [15], which corrects syntax errors in speech recognition hypotheses, was built in order to enhance vocal Human-Robot Interaction and to enhance the previously developed model [40]. Additionally, the ability to deal with several languages (from different language families) of this later model of sentence parsing [40] was evaluated. We showed that it can successfully learn to parse sentences related to home scenarios in fifteen languages originating from Europe and Asia [24]. In a different perspective, in order to try to overcome word misrecognition at a more basic level, we tested whether the same architecture was able to process directly phonemes instead of grammatical constructions [17]. Applied on a small corpus, we see that the model has similar performance.

In an industrial application for the representation of electrical diagrams (cf. § 8.1), we also study how recurrent layered models can be trained to run through these schemes for prediction and sequence representation tasks [10].

The second paradigm concerns the extraction of characteristics and the use of hierarchical networks, as in the case of deep networks. An industrial application (cf. § 9.2) allows us to revisit these models to make them more easily usable in constrained frameworks, for example with limited size corpuses, and more interpretable introducing a new notion of prototypes and exploring the capability to learn the network architecture itself (using shortcuts) [11]. In order to push the state of the art, the next step is going to consider not only feed-forward but also recurrent architecture, and to this end neural network recurrent weight estimation through backward tuning has been revisited [21].

The third paradigm is about spatial computation. We have designed a graphical method originating from the computer graphics domain that is used for the arbitrary and intuitive placement of cells over a two-dimensional manifold. Using a bitmap image as input, where the color indicates the identity of the different structures and the alpha channel indicates the local cell density, this method guarantees a discrete distribution of cell position respecting the local density function. This method scales to any number of cells, allows to specify several different structures at once with arbitrary shapes and provides a scalable and versatile alternative to the more classical assumption of a uniform non-spatial distribution. This preliminary work will be used in the design of a new class of model where explicit topography allows to connect structure according to known pathways.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Contract with Algotech

Participants: Frédéric Alexandre, Ikram Chraibi Kaadoud, Nicolas Rougier, Thierry Viéville.

Algotech is a SME working in the domain of CADD software edition for electrical circuit diagram interpretation and design. Its activity is interesting for our team because they are also interested in the design, by learning, of perception (for diagram identification) and action aspects of loops (for diagram genesis) with the specificity of working at a small scale, considering the variety of items to be manipulated. This is consequently a very interesting benchmark for transferring our bio-inspired models to the domain of classical machine learning.
9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. PsyPhINe

**Participant:** Nicolas Rougier.

Project gathering researchers from: MSH Lorraine (USR3261), InterPsy (EA 4432), APEMAC, EPSaM (EA4360), Archives Henri-Poincaré (UMR7117), Loria (UMR7503) & Mnemosyne.

PsyPhiNe is a pluridisciplinary and exploratory project between philosophers, psychologists, neuroscientists and computer scientists. The goal of the project is to explore cognition and behavior from different perspectives. The project aims at exploring the idea of assignments of intelligence or intentionality, assuming that our intersubjectivity and our natural tendency to anthropomorphize play a central role: we project onto others parts of our own cognition. To test these hypotheses, we ran a series of experiments with human subject confronted to a motorized lamp that can or cannot interact with them while they’re doing a specific task. We’ve organized our third national conference in Nancy gathering speakers from philosophy, robotics, art and psychology and closed a three years cycle. The group now aims at publishing a book gathering text from all the invited speakers.

9.2. National Initiatives

9.2.1. FUI Sumatra

**Participants:** Frédéric Alexandre, Thalita Firmo Drumond, Xavier Hinaut, Randa Kassab, Nicolas Rougier, Thierry Viéville.

This FUI project, supported by the Aerospace Valley Innovation Pole, gathers two industrial groups (Safran Helicopter and SPIE), three research labs and four SME. Its goal is to provide contextualized information to maintenance operators by the online analysis of the operating scene. We are concerned in this project with the analysis of visual scenes, in industrial contexts, and the extraction of visual primitives, categories and pertinent features, best decribing the scenes, with biologically inspired neuronal models.

Firstly, this is an opportunity for us to revisit the principles of deep network architectures by adapting principles that we will elaborate from the context of the hierarchical architecture of the temporal visual cortex. Secondly, we intend to exploit and adapt our model of hippocampus to extract more heterogenous features. This project is an excellent opportunity to associate and combine our models and also to evaluate the robustness of our models in real-world applications.

9.2.2. ANR SOMA (PRCI)

**Participant:** Nicolas Rougier.

This new project is a convergence point between past research approaches toward new computational paradigms: adaptive reconfigurable architecture, cellular computing, computational neuroscience, and neuromorphic hardware:

1. SOMA is an adaptive reconfigurable architecture to the extent that it will dynamically re-organize both its computation and its communication by adapting itself to the data to process.
2. SOMA is based on cellular computing since it targets a massively parallel, distributed and decentralized neuromorphic architecture.
3. SOMA is based on computational neuroscience since its self-organization capabilities are inspired from neural mechanisms.
4. SOMA is a neuromorphic hardware system since its organization emerges from the interactions between neural maps transposed into hardware from brain observation.
This project represents a significant step toward the definition of a true fine-grained distributed, adaptive and
decentralized neural computation framework. Using self-organized neural populations onto a cellular machine
where local routing resources are not separated from computational resources, it will ensure natural scalability
and adaptability as well as a better performance/power consumption tradeoff compared to other conventional
embedded solutions.

9.2.3. ANR MACAQUE40
Participant: Nicolas Rougier.

Most of the theoretical models in economics proposed so far to describe money emergence are based on three
intangible assumptions: the omniscience of economic agents, an infinite time and an extremely large number
of agents (not bounded). The goal of this interdisciplinary study is to investigate the condition of apparition of
a monetary economy in a more ecological framework provided with the assumption that the market is made
up of a finite number of agents having a bounded rationality and facing a time constraint.

In this study, we propose a generic model and environment of monetary prospecting. Our first objective is to
artificially identify structural (trading organisation, agents specialisation) and cognitive conditions (learning
skills, memory and strategic anticipation abilities, tradeoff exploration/exploitation) that allowed money
emergence. This will provide relevant environmental constraints that we will use during our manipulations
in the laboratory. The agents that will be involved in these manipulations will be of two types: non-human
primates (rhesus macaques) and humans.

9.2.4. Project Motus of the ANSES
Participant: André Garenne.

The MOTUS project (MOdulaTion dU Signal RF et effets sur le cerveau : approche in vivo et in vitro) is
financed by the ANSES (the french national agency for health security). This 3 years project is studying the
effects of GSM-RF on living matter and especially neuronal activity and development. Our main involvement
cornsells electrophysiological data and spike trains analysis as well as the development of pharmacological
protocols to test GSM-RF effects hypotheses.

This year, we have designed and realised new experiments in order to better characterize the effect of 1800 Mz
RF field of GSM on the spontaneous activity of in-vitro cortical cell cultures. In the current study, our aim was
to highlight a dose-response relationship for this effect. To do this, we have recorded the spontaneous bursting
activity of cortical neurons cultures on multi-electrodes arrays. We have thus shown that at SAR (Specific
Absorption Rate) ranging from 0.01 to 9.2 W/kg the signal elicited a clear decrease in bursting rate during
the RF exposure phase that lasted even after the end of the exposure. Moreover, the effect grew larger with
increasing SAR, and the amplitude of the change was greater with a GSM signal than with a continuous wave
RF field of the same energy level. These experimental findings provide evidence for clear effects of RF signals
on the bursting rate of neuronal cultures.

9.3. International Initiatives

9.3.1. Inria Associate Teams Not Involved in an Inria International Labs

9.3.1.1. Braincraft
Title: Braincraft

International Partner (Institution - Laboratory - Researcher):
University of Colorado, Boulder (United States) - Computational Cognitive Neuroscience
- Randall O’Reilly
What are the processes by which animals and humans select their actions based on their motivations and on the consequences of past actions? This is a fundamental question in neurosciences, with implications to ethology, psychology, economics, sociology and computer science. Through a unique combination of expertise in cognitive psychology, neurosciences and computer science, this associate team will foster a collaboration for developing a computationally-based understanding of the neural circuits involved in decision making, namely basal ganglia and prefrontal cortex. One of the key question is to know the overall contribution of these structures and their function in the decision process.

9.3.2. Participation in Other International Programs

9.3.2.1. Project LingoRob with Germany

LingoRob - Learning Language in Developmental Robots - is a project of the Programme Hubert Curien PHC Procope with Germany (University of Hamburg). The scientific objective of the collaboration is to better understand the mechanisms underlying language acquisition and enable more natural interaction between humans and robots in different languages, while modelling how the brain processes sentences and integrates semantic information of scenes. Models developed in both labs involve artificial neural networks, and in particular Echo State Networks (ESN), also known as pertaining to the Reservoir Computing framework. These neural models allow insights on high-level processes of the human brain, and at the same time are well suited as robot control platform, because they can be trained and executed online with low computational resources. The collaborators will also combine Deep Learning networks to the reservoir models already used in order to benefit from their very good feature extraction abilities.

9.3.2.2. Project BGaL with India

In the 3-years project “Basal Ganglia at Large (BGaL)”, funded by the CNRS and the CEFIPRA, we collaborate with the computer science department of IIT Hyderabad and the biomedical department of IIT Madras, for the design of models of basal ganglia and for their implementation at large scale as well as for their relation with other brain structures. This year we have worked on a model of a dopaminergic region, VTA, central for reinforcement learning in the basal ganglia.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

Prof. Chakravarthy Srinivasa
Date: Nov-Dec 2017
Institution: IIT Madras, Chennai (India)

Johannes Twiefel
Date: 10 days, Sep 2017; 1 week, Nov 2017.
Institution: University of Hamburg, Germany.

Luiza Mici
Date: 10 days, Sep 2017.
Institution: University of Hamburg, Germany.

9.4.1.1. Internships

Remya Sankar
Date: June 2017 - Dec 2017
Institution: IIIT Hyderabad (India)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

10.1.1.2. Member of the Organizing Committees
F. Alexandre: organization of the Latin-American Summer School on Computational Neuroscience (Laconeu, 9-27 January 2017, Valparaiso, Chile).

10.1.2. Scientific Events Selection
10.1.2.1. Member of the Conference Program Committees

10.1.2.2. Reviewer
- F. Alexandre: NER’17; ICDL-EPIROB 2017;
- Nicolas Rougier: Frontiers in Computational Neuroscience, Complexity, JOSS, ReScience;
- X. Hinaut: CogSci’17, ICDL-EPIROB 2017, ESANN 2018;

10.1.3. Journal
10.1.3.1. Member of the Editorial Boards
- Frédéric Alexandre: Review Editor for Frontiers in Neurorobotics;

10.1.3.2. Reviewer - Reviewing Activities
- F. Alexandre: Frontiers in Neuroscience; PLoS ONE; Cognitive Computation; Nature Scientific Reports; eLife;
- André Garenne: Journal of Integrative Neuroscience

10.1.4. Invited Talks
F. Alexandre:
- Workshop on Computational Neuroscience: New trends and challenges for 2030; January 18, Valparaiso, Chile.
- 2017 meeting of the GDR Neurosciences of memory NeuroMem, May, 16.
- Seminar “Modeling Cognitive Processes” of the laboratory LEAD, Dijon (Nov. 24).
- Annual meeting of the AMAF medical association (“Modeling Cognitive Functions and Artificial Intelligence”, Nov. 25, Creteil).

Nicolas Rougier:
- Lex Robotica, Paris, France
- 7th Symposium on the Biology of Decision Making, Bordeaux, France
- Open Science, Bordeaux, France
- Scientific Python, La Rochelle, France
- Reproduction is not replication, Reading, UK

X. Hinaut:
- Workshop "The role of the basal ganglia in the interaction between language and other cognitive functions", DEC, ENS Ulm, October 12-13, Paris, France.
10.1.5. Leadership within the Scientific Community

X. Hinaut:
- President of the association MindLaBDX: “open citizen lab” in Cognitive Sciences and Artificial Intelligence in Bordeaux.
- member of the Administration Committee of Fresco association (French Federation of students in Cognitive Science)

Nicolas Rougier: Editor in chief for ReScience

10.1.6. Scientific Expertise

F. Alexandre is the french expert for Mathematics and Computer Science of the PHC (Hubert Curien Program) Utique for scientific cooperation between France and Tunisia. In 2017, he participated to the CHIST ERA Evaluation Panel, May 18-19 and acted as an expert for the ANR.

10.1.7. Research Administration

- F. Alexandre is member of the Inria Evaluation Committee; Deputy Scientific Delegate and Vice-head of the Project Committee of Inria Bordeaux Sud-Ouest; Corresponding scientist for Bordeaux Sud-Ouest of the Inria COERLE ethical committee; Member of the national Inria committee for international chairs; Member of the local Inria committee for young researchers hiring; Member of the steering committee of the regional Cluster on Information Technology and Health; of the regional Cluster on Robotics; Expert of the ITMO ‘Neurosciences, Sciences Cognitive, Neurologie, Psychiatrie’
- N. Rougier is vice-head of the Mnemosyne team-project; elected member of the Inria Evaluation Committee; Responsible of the local Inria committee for invited professors; Member of the steering committee for the BioComp CNRS consortium; Editor in chief and co-founder of ReScience.
- Thierry Viéville is in charge of the http://classcode.fr project and in charge, for Inria, of the creation of a Master SmartEdTech at UCA within the scope of his mission for the Inria Sophia Antipolis - Méditérannée direction.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

F. Alexandre: teaching at the Laconeu summer school 9-27 january 2017, Valparaiso, Chile. Teaching Ethics for Inria PhD students (Sept. 25 and Oct. 6).

André Garenne (in collaboration with Xavier Nogues) created a new teaching unit for bachelor students in biology at the final stage of their graduation. This unit will be half dedicated to the learning of programming basics using Python and its scientific libraries and half dedicated to the learning of statistical data analysis methods relying mainly on machine learning approaches and the R language.

Nicolas Rougier organized a python scientific course (24h) for the doctoral students in mathematics and computer science.

Thierry Viéville is since 2009 in charge of formations of high-school teachers in popular computer science and taught computational neuroscience in the Master of Cognitive Science and Ergonomics.

In addition, many courses are given in french universities and schools of engineers at different levels (LMD) by most team members, in computer science, in applied mathematics, in neuroscience and in cognitive science.
10.2.2. Juries

We participate to many juries each year.

10.3. Popularization

For a multi-disciplinary team as Mnemosyne, science popularization is not only a nice and useful contribution to the dissemination of scientific knowledge but also a necessity since we work with colleagues from biosciences with whom sharing profound ideas in computer science is mandatory for a real collaboration.

- Thierry Viéville is for 50% of his time involved in popularization actions, mainly computer science large audience education, and has been promoted Officer of the Order of Academic Palms for the collective contribution of the Inria Science Outreach mission.
- F. Alexandre organized a conference about artificial intelligence with high-school children (Sept. 28, Lormont)
- I. Chraibi Kaadoud participated to the regional challenge: “My PhD in 180 seconds”
- X. Hinaut organized the 1st hackathon of Bordeaux in Cognitive Sciences and Artificial Intelligence, 8-10 December, Cap Sciences, Bordeaux. (https://mindlabdx.github.io/hack1cerveau/); Organization of a workshop on cellular automaton at Le Node, Bordeaux; Meeting groups of high-school students for their projects on Artificial Intelligence topics.

11. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journal


Invited Conferences


International Conferences with Proceedings


[12] P. S. KAUSHIK, M. S. CARRERE, F. ALEXANDRE, S. B. RAJU, A biologically inspired neuronal model of reward prediction error computation, in "IJCNN 2017 - International Joint Conference on Neural Networks", Anchorage, United States, May 2017, 8, https://hal.inria.fr/hal-01528658.


Conferences without Proceedings


**Scientific Books (or Scientific Book chapters)**


**Research Reports**


**Scientific Popularization**


**Other Publications**


References in notes


Project-Team MONC

Mathematical modeling for Oncology

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS
Institut Polytechnique de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences
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Project-Team MONC

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 November 01

Keywords:

**Computer Science and Digital Science:**
- A6.1. - Mathematical Modeling
- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.4. - Multiscale modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.2.4. - Statistical methods
- A6.2.6. - Optimization
- A6.2.7. - High performance computing
- A6.3.1. - Inverse problems
- A6.3.2. - Data assimilation
- A6.3.3. - Data processing
- A6.3.4. - Model reduction

**Other Research Topics and Application Domains:**
- B1.1.9. - Bioinformatics
- B1.1.10. - Mathematical biology
- B1.1.11. - Systems biology
- B2.2.3. - Cancer
- B2.4.2. - Drug resistance
- B2.6.1. - Brain imaging
- B2.6.3. - Biological Imaging

1. Personnel

**Research Scientists**
- Olivier Saut [Team leader, CNRS, Researcher, HDR]
- Sebastien Benzekry [Inria, Researcher, HDR]
- Amandine Crombe [Institut Bergonié, Researcher, from Nov 2017]
- Baudouin Denis de Senneville [CNRS, Researcher, from May 2017, HDR]
- Clair Poignard [Inria, Researcher, HDR]

**Faculty Members**
- Thierry Colin [Institut National Polytechnique de Bordeaux, Professor, HDR]
- Annabelle Collin [Institut National Polytechnique de Bordeaux, Associate Professor]

**External Collaborators**
- Mikaël Antoine [Institut Bergonié]
- Baudouin Denis de Senneville [CNRS, until Apr 2017, HDR]
- Louise Missenard [Institut Bergonié]
- Vivien Pianet [Univ de Bordeaux, until Feb 2017]
- Claudia Pouypoudat [CHU Bordeaux]
- Benjamin Taton [Univ de Bordeaux]

**Technical Staff**
2. Overall Objectives

2.1. Objectives

The MONC project-team aims at developing new mathematical models built on partial differential equations and statistical methods and based on precise biological and medical knowledge. The goal is ultimately to be able to help clinicians and/or biologists to better understand, predict or control tumor growth and possibly evaluate the therapeutic response, in a clinical context or for pre-clinical studies through quantitative numerical tools. We develop patient-specific approaches (mainly based on medical images) as well as population-type approaches in order to take advantage of large databases. We claim that we can have a clinical impact that can change the way of handling certain pathologies.

In vivo modeling of tumors is limited by the amount of information obtainable. However, recently, there have been dramatic increases in the scope and quality of patient-specific data from non-invasive imaging methods, so that several potentially valuable measurements are now available to quantitatively measure tumor growth, assess tumor status as well as anatomical or functional details. Using different techniques such as CT scan, magnetic resonance imaging (MRI), or positron emission tomography (PET), it is now possible to evaluate and define tumor status at different levels or scales: physiological, molecular and cellular.

In the meantime, the understanding of the biological mechanisms of tumor growth, including the influence of the micro-environment, has greatly increased and medical doctors now have access to a wide spectrum of therapies (surgery, mini-invasive techniques, radiotherapies, chemotherapies, targeted therapies...).
Our project aims at supporting the decision process of oncologists in the definition of therapeutic protocols via quantitative methods. The idea is to build phenomenological mathematical models based on data obtained in the clinical imaging routine like CT scans, MRIs and PET scans. We therefore want to offer medical doctors patient-specific tumor growth models, which are able to evaluate – on the basis of previously collected data and within the limits of phenomenological models – the time evolution of the pathology at subsequent times and the response to therapies. More precisely, our goal is to help clinicians answer the following questions thanks to our numerical tools:

1. When is it necessary to start a treatment?
2. What is the best time to change a treatment?
3. When to stop a treatment?

In addition, we also intend to incorporate real-time model information for improving the accuracy and efficacy of non invasive or micro-invasive tumor ablation techniques like acoustic hyperthermia, electroporation, radiofrequency, cryo-ablation and of course radiotherapies.

There is therefore a critical need of integrating biological knowledge into mathematical models based on clinical or experimental data. The main purpose of our project is to create new mathematical models and new paradigms for data assimilation that are adapted to the biological nature of the disease and to the amount of multi-modal data available.

### 2.2. General strategy

![3D numerical simulation of a meningioma. The tumor is shown in red.](image)

The general strategy consists of the interactions of several stages:

- **Stage 1:** Derivation of mechanistic models based on the biological knowledge and the available observations. The construction of such models relies on the up-to-date biological knowledge at the cellular level including description of the cell-cycle, interaction with the microenvironment (angiogenesis, interaction with the stroma). Such models also include a “macroscopic” description of specific molecular pathways that are known to have a critical role in carcinogenesis or that are targeted by new drugs. We emphasize that for this purpose, close interactions with biologists are crucial. Lots of works devoted to modeling at the cellular level are available in the literature. However, in order to be able to use these models in a clinical context, the tumor is also to be described at the tissue level. The *in vitro* mechanical characterization of tumor tissues has been
It is therefore necessary to build adapted phenomenological models, according to the biological and clinical reality.

- **Stage 2: Data collection.** In the clinical context, data may come from medical imaging (MRI, CT-Scan, PET scan) at different time points. It is also a crucial point: we need longitudinal data in time in order to be able to understand the evolution of the disease. Data may also be obtained from analyses of blood samples or biopsies. A close collaboration with clinicians is required for selecting the specific cases to focus on, the understanding of the key points and data, the classification of the grades of the tumors, the understanding of the treatment... In the preclinical context, data may for instance be macroscopic measurements of the tumor volume for subcutaneous cases, green fluorescence protein (GFP) quantifications for total number of living cells, non-invasive bioluminescence signals or even imaging obtained with devices adapted to small animals.
  - **Data processing:** Besides selection of representative cases by our collaborators, most of the time, data has to be processed before being used in our models. We develop novel methods for semi-automatic segmentations (they are implemented in SegmentIt), non-rigid registration and extraction of image texture information.

- **Stage 3: Adaptation of the model to data.** The model has to be adapted to data: it is useless to have a model taking many biological features of the disease into account if it cannot be reliably parameterized with available data. For example, very detailed descriptions of the angiogenesis process found in the literature cannot be used, as they have too much parameters to determine for the information available. A pragmatic approach has to be developed for this purpose. On the other hand, one has to try to model any element that can be useful to exploit the image. Parameterizing must be performed carefully in order to achieve an optimal trade-off between the accuracy of the model, its complexity, identifiability and predictive power. Parameter estimation is a critical issue in mathematical biology: if there are too many parameters, it will be impossible to estimate them but if the model is too simple, it will be too far from reality.

- **Stage 4: Data assimilation.** Because of data complexity - for example multimodal, longitudinal medical imaging - data assimilation is a major challenge. Such a process is a combination of methods for solving inverse problems and statistical methods including machine learning strategies.
– Personalized models: Currently, most of the inverse problems developed in the team are solved using a gradient method coupled with some MCMC type algorithm. We are now trying to use more efficient methods as Kalman type filters or so-called Luenberger filter (nudging). Using sequential methods could also simplify Stage 3 because they can be used even with complex models. Of course, the strategy used by the team depends on the quantity and the quality of data. It is not the same if we have an homogeneous population of cases or if it is a very specific isolated case.

– Statistical learning: In some clinical cases, there is no longitudinal data available to build a mathematical model describing the evolution of the disease. In these cases (e.g. in our collaboration with Humanitas Research Hospital), we use machine learning techniques to correlate clinical and imaging features with clinical outcome of patients (radiomics). When longitudinal data and a sufficient number of patients are available, we combine this approach and mathematical modeling by adding the personalized model parameters for each patient as features in the statistical algorithm. Our goal is then to have a better description of the evolution of the disease over time (as compared to only taking temporal variations of features into account). We also plan to use statistical algorithms to build reduced-order models, more efficient to run or calibrate than the original models.

– Data assimilation of gene expression. "Omics" data become more and more important in oncology and we aim at developing our models using this information as well. For example, in our work on GIST, we have taken the effect of a Ckit mutation on resistance to treatment into account. However, it is still not clear how to use in general gene expression data in our macroscopic models, and particularly how to connect the genotype to the phenotype and the macroscopic growth. We expect to use statistical learning techniques on populations of patients in order to move towards this direction, but we emphasize that this task is very prospective and is a scientific challenge in itself.

• Stage 5: Simulation and prediction. Once the models have been parametrized, the simulation part can be done. We also need to include a quantification of uncertainties and to produce 3D simulations that can be confronted to reality.

3. Research Program

3.1. Introduction

We are working in the context of data-driven medicine against cancer. We aim at coupling mathematical models with data to address relevant challenges for biologists and clinicians in order for instance to improve our understanding in cancer biology and pharmacology, assist the development of novel therapeutic approaches or develop personalized decision-helping tools for monitoring the disease and evaluating therapies.

More precisely, our research on mathematical oncology is three-fold:

• Axis 1: Tumor modeling for patient-specific simulations: Clinical monitoring. Numerical markers from imaging data. Radiomics.

• Axis 2: Bio-physical modeling for personalized therapies: Electroporation from cells to tissue. Radiotherapy.

• Axis 3: Quantitative cancer modeling for biological and preclinical studies: Biological mechanisms. Metastatic dissemination. Pharmacometrics.

In the first axis, we aim at producing patient-specific simulations of the growth of a tumor or its response to treatment starting from a series of images. We hope to be able to offer a valuable insight on the disease to the clinicians in order to improve the decision process. This would be particularly useful in the cases of relapses or for metastatic diseases.
Figure 3. General strategy of the team to build meaningful models in oncology.
The second axis aims at modeling biophysical therapies like radiotherapies, but also thermo-ablations, radiofrequency ablations or electroporation that play a crucial role in the case of a relapse or for a metastatic disease, which is precisely the clinical context where the techniques of axis 1 will be applied.

The third axis, even if not directly linked to clinical perspectives, is essential since it is a way to better understand and model the biological reality of cancer growth and the (possibly complex) effects of therapeutic intervention. Modeling in this case also helps to interpret the experimental results and improve the accuracy of the models used in Axis 1. Technically speaking, some of the computing tools are similar to those of Axis 1.

3.2. Axis 1: Tumor modeling for patient-specific simulations

The gold standard treatment for most cancers is surgery. In the case where total resection of the tumor is possible, the patient often benefits from an adjuvant therapy (radiotherapy, chemotherapy, targeted therapy or a combination of them) in order to eliminate the potentially remaining cells that may not be visible. In this case personalized modeling of tumor growth is useless and statistical modeling will be able to quantify the risk of relapse, the mean progression-free survival time...However if total resection is not possible or if metastases emerge from distant sites, clinicians will try to control the disease for as long as possible. A wide set of tools are available. Clinicians may treat the disease by physical interventions (radiofrequency ablation, cryoablation, radiotherapy, electroporation, focalized ultrasound,...) or chemical agents (chemotherapies, targeted therapies, antiangiogenic drugs, immunotherapies, hormonotherapies). One can also decide to monitor the patient without any treatment (this is the case for slowly growing tumors like some metastases to the lung, some lymphomas or for some low grade glioma). A reliable patient-specific model of tumor evolution with or without therapy may have different uses:

- **Case without treatment:** the evaluation of the growth of the tumor would offer a useful indication for the time at which the tumor will reach a critical size. For example, radiofrequency ablation of pulmonary lesion is very efficient as long as the diameter of the lesion is smaller than 3 cm. Thus, the prediction can help the clinician plan the intervention. For slowly growing tumors, quantitative modeling can also help to decide at what time interval the patient has to undergo a CT-scan. CT-scans are irradiative exams and there is a challenge for decreasing their occurrence for each patient. It has also an economical impact. And if the disease evolution starts to differ from the prediction, this might mean that some events have occurred at the biological level. For instance, it could be the rise of an aggressive phenotype or cells that leave a dormancy state. This kind of events cannot be predicted, but some mismatch with respect to the prediction can be an indirect proof of their existence. It could be an indication for the clinician to start a treatment.

- **Case with treatment:** a model can help to understand and to quantify the final outcome of a treatment using the early response. It can help for a redefinition of the treatment planning. Modeling can also help to anticipate the relapse by analyzing some functional aspects of the tumor. Again, a deviation with respect to reference curves can mean a lack of efficiency of the therapy or a relapse. Moreover, for a long time, the response to a treatment has been quantified by the RECIST criteria which consists in (roughly speaking) measuring the diameters of the largest tumor of the patient, as it is seen on a CT-scan. This criteria is still widely used and was quite efficient for chemotherapies and radiotherapies that induce a decrease of the size of the lesion. However, with the systematic use of targeted therapies and anti-angiogenic drugs that modify the physiology of the tumor, the size may remain unchanged even if the drug is efficient and deeply modifies the tumor behavior. One better way to estimate this effect could be to use functional imaging (Pet-scan, perfusion or diffusion MRI, ...), a model can then be used to exploit the data and to understand in what extent the therapy is efficient.

- **Optimization:** currently, we do not believe that we can optimize a particular treatment in terms of distribution of doses, number, planning with the model that we will develop in a medium term perspective. But it is an aspect that we keep in mind on a long term one.
The scientific challenge is therefore as follows: knowing the history of the patient, the nature of the primitive tumor, its histopathology, knowing the treatments that patients have undergone, knowing some biological facts on the tumor and having a sequence of images (CT-scan, MRI, PET or a mix of them), are we able to provide a numerical simulation of the extension of the tumor and of its metabolism that fits as best as possible with the data (CT-scans or functional data) and that is predictive in order to address the clinical cases described above?

Our approach relies on the elaboration of PDE models and their parametrization with the image by coupling deterministic and stochastic methods. The PDE models rely on the description of the dynamics of cell populations. The number of populations depends on the pathology. For example, for glioblastoma, one needs to use proliferative cells, invasive cells, quiescent cells as well as necrotic tissues to be able to reproduce realistic behaviors of the disease. In order to describe the relapse for hepatic metastases of gastro-intestinal stromal tumor (gist), one needs three cell populations: proliferative cells, healthy tissue and necrotic tissue.

The law of proliferation is often coupled with a model for the angiogenesis. However such models of angiogenesis involve too many non measurable parameters to be used with real clinical data and therefore one has to use simplified or even simplistic versions. The law of proliferation often mimics the existence of an hypoxia threshold, it consists of an ODE, or a PDE that describes the evolution of the growth rate as a combination of sigmoid functions of nutrients or roughly speaking oxygen concentration. Usually, several laws are available for a given pathology since at this level, there are no quantitative argument to choose a particular one.

The velocity of the tumor growth differs depending on the nature of the tumor. For metastases, we will derive the velocity thanks to Darcy’s law in order to express that the extension of the tumor is basically due to the increase of volume. This gives a sharp interface between the metastasis and the surrounding healthy tissues, as observed by anatomopathologists. For primitive tumors like glioma or lung cancer, we use reaction-diffusion equations in order to describe the invasive aspects of such primitive tumors.

The modeling of the drugs depends on the nature of the drug: for chemotherapies, a death term can be added into the equations of the population of cells, while antiangiogenic drugs have to be introduced in a angiogenic model. Resistance to treatment can be described either by several populations of cells or with non-constant growth or death rates. As said before, it is still currently difficult to model the changes of phenotype or mutations, we therefore propose to investigate this kind of phenomena by looking at deviations of the numerical simulations compared to the medical observations.

The calibration of the model is achieved by using a series (at least 2) of images of the same patient and by minimizing a cost function. The cost function contains at least the difference between the volume of the tumor that is measured on the images with the computed one. It also contains elements on the geometry, on the necrosis and any information that can be obtained through the medical images. We will pay special attention to functional imaging (PET, perfusion and diffusion MRI). The inverse problem is solved using a gradient method coupled with some Monte-Carlo type algorithm. If a large number of similar cases is available, one can imagine to use statistical algorithms like random forests to use some non quantitative data like the gender, the age, the origin of the primitive tumor...for example for choosing the model for the growth rate for a patient using this population knowledge (and then to fully adapt the model to the patient by calibrating this particular model on patient data) or for having a better initial estimation of the modeling parameters. We have obtained several preliminary results concerning lung metastases including treatments and for metastases to the liver.

3.3. Axis 2: Bio-physical modeling for personalized therapies

In this axis, we investigate locoregional therapies such as radiotherapy, irreversible electroporation. Electroporation consists in increasing the membrane permeability of cells by the delivery of high voltage pulses. This non-thermal phenomenon can be transient (reversible) or irreversible (IRE). IRE or electro-chemotherapy – which is a combination of reversible electroporation with a cytotoxic drug – are essential tools for the treatment of a metastatic disease. Numerical modeling of these therapies is a clear scientific challenge. Clinical applications of the modeling are the main target, which thus drives the scientific approach, even though theoretical studies in order to improve the knowledge of the biological phenomena, in particular for electroporation,
should also be addressed. However, this subject is quite wide and we focus on two particular approaches: some aspects of radiotherapies and electro-chemotherapy. This choice is motivated partly by pragmatic reasons: we already have collaborations with physicians on these therapies. Other treatments could be probably treated with the same approach, but we do not plan to work on this subject on a medium term.

- **Radiotherapy (RT)** is a common therapy for cancer. Typically, using a CT scan of the patient with the structures of interest (tumor, organs at risk) delineated, the clinicians optimize the dose delivery to treat the tumor while preserving healthy tissues. The RT is then delivered every day using low resolution scans (CBCT) to position the beams. Under treatment the patient may lose weight and the tumor shrinks. These changes may affect the propagation of the beams and subsequently change the dose that is effectively delivered. It could be harmful for the patient especially if sensitive organs are concerned. In such cases, a replanification of the RT could be done to adjust the therapeutical protocol. Unfortunately, this process takes too much time to be performed routinely. The challenges faced by clinicians are numerous, we focus on two of them:

  - **Detecting the need of replanification**: we are using the positioning scans to evaluate the movement and deformation of the various structures of interest. Thus we can detect whether or not a structure has moved out of the safe margins (fixed by clinicians) and thus if a replanification may be necessary. In a retrospective study, our work can also be used to determine RT margins when there are no standard ones. A collaboration with the RT department of Institut Bergonié is underway on the treatment of retroperitoneal sarcoma and ENT tumors (head and neck cancers). A retrospective study was performed on 11 patients with retro-peritoneal sarcoma. The results have shown that the safety margins (on the RT) that clinicians are currently using are probably not large enough. The tool used in this study was developed by an engineer funded by Inria (Cynthia Périer, ADT Sesar). We used well validated methods from a level-set approach and segmentation / registration methods. The originality and difficulty lie in the fact that we are dealing with real data.

![Figure 4. Plot showing the accuracy of our prediction on meningioma volume. Each point corresponds to a patient whose two first exams were used to calibrate our model. A patient-specific prediction was made with this calibrated model and compared with the actual volume as measured on a third time by clinicians. A perfect prediction would be on the black dashed line. Medical data was obtained from Prof. Loiseau, CHU Pellegrin.](image-url)
in a clinical setup. Clinicians have currently no way to perform complex measurements with their clinical tools. This prevents them from investigating the replanification. Our work and the tools developed pave the way for easier studies on evaluation of RT plans in collaboration with Institut Bergonié. *There was no modeling involved in this work that arose during discussions with our collaborators.* The main purpose of the team is to have meaningful outcomes of our research for clinicians, sometimes it implies leaving a bit our area of expertise.

- **Evaluating RT efficacy and finding correlation between the radiological responses and the clinical outcome:** our goal is to help doctors to identify correlation between the response to RT (as seen on images) and the longer term clinical outcome of the patient. Typically, we aim at helping them to decide when to plan the next exam after the RT. For patients whose response has been linked to worse prognosis, this exam would have to be planned earlier. This is the subject of collaborations with Institut Bergonié and CHU Bordeaux on different cancers (head and neck, pancreas). The response is evaluated from image markers (*e.g.* using texture information) or with a mathematical model developed in Axis 1. The other challenges are either out of reach or not in the domain of expertise of the team. Yet our works may tackle some important issues for adaptive radiotherapy.

- **Both IRE and electrochemotherapy** are anticancerous treatments based on the same phenomenon: the electroporation of cell membranes. This phenomenon is known for a few decades but it is still not well understood, therefore our interest is two fold:

  1. We want to use mathematical models in order to better understand the biological behavior and the effect of the treatment. We work in tight collaboration with biologists and bioelectromagneticians to derive precise models of cell and tissue electroporation, in the continuity of the research program of the Inria team-project MC2. These studies lead to complex non-linear mathematical models involving some parameters (as less as possible). Numerical methods to compute precisely such models and the calibration of the parameters with the experimental data are then addressed. Tight collaborations with the Vectoro-logy and Anticancerous Therapies (VAT) of IGR at Villejuif, Laboratoire Ampère of Ecole Centrale Lyon and the Karlsruhe Institute of technology will continue, and we aim at developing new collaborations with Institute of Pharmacology and Structural Biology (IPBS) of Toulouse and the Laboratory of Molecular Pathology and Experimental Oncology (LMPEO) at CNR Rome, in order to understand differences of the electroporation of healthy cells and cancer cells in spheroids and tissues.

  2. This basic research aims at providing new understanding of electroporation, however it is necessary to address, particular questions raised by radio-oncologists that apply such treatments. One crucial question is “What pulse or what train of pulses should I apply to electroporate the tumor if the electrodes are located as given by the medical images”? Even if the real-time optimization of the placement of the electrodes for deep tumors may seem quite utopian since the clinicians face too many medical constraints that cannot be taken into account (like the position of some organs, arteries, nerves...), one can expect to produce real-time information of the validity of the placement done by the clinician. Indeed, once the placement is performed by the radiologists, medical images are usually used to visualize the localization of the electrodes. Using these medical data, a crucial goal is to provide a tool in order to compute in real-time and visualize the electric field and the electroporated region directly on these medical images, to give the doctors a precise knowledge of the region affected by the electric field. In the long run, this research will benefit from the knowledge of the theoretical electroporation modeling, but it seems important to use the current knowledge of tissue electroporation – even quite rough –, in order to rapidly address the specific difficulty of such a goal (real-time computing of non-linear model, image segmentation and visualization). Tight collaborations with CHU Pellegrin at Bordeaux, and CHU J. Verdier at Bondy are crucial.
- **Radiofrequency ablation.** In a collaboration with Hopital Haut Leveque, CHU Bordeaux we are trying to determine the efficacy and risk of relapse of hepatocellular carcinoma treated by radiofrequency ablation. For this matter we are using geometrical measurements on images (margins of the RFA, distance to the boundary of the organ) as well as texture information to statistically evaluate the clinical outcome of patients.

- **Intensity focused ultrasound.** In collaboration with Utrecht Medical center, we aim at tackling several challenges in clinical applications of IFU: target tracking, dose delivery...

### 3.4. Axis 3: Quantitative cancer modeling for biological and preclinical studies

With the emergence and improvement of a plethora of experimental techniques, the molecular, cellular and tissue biology has operated a shift toward a more quantitative science, in particular in the domain of cancer biology. These quantitative assays generate a large amount of data that call for theoretical formalism in order to better understand and predict the complex phenomena involved. Indeed, due to the huge complexity underlying the development of a cancer disease that involves multiple scales (from the genetic, intra-cellular scale to the scale of the whole organism), and a large number of interacting physiological processes (see the so-called "hallmarks of cancer"), several questions are not fully understood. Among these, we want to focus on the most clinically relevant ones, such as the general laws governing tumor growth and the development of metastases (secondary tumors, responsible of 90% of the deaths from a solid cancer). In this context, it is thus challenging to exploit the diversity of the data available in experimental settings (such as *in vitro* tumor spheroids or *in vivo* mice experiments) in order to improve our understanding of the disease and its dynamics, which in turn lead to validation, refinement and better tuning of the macroscopic models used in the axes 1 and 2 for clinical applications.

In recent years, several new findings challenged the classical vision of the metastatic development biology, in particular by the discovery of organism-scale phenomena that are amenable to a dynamical description in terms of mathematical models based on differential equations. These include the angiogenesis-mediated distant inhibition of secondary tumors by a primary tumor the pre-metastatic niche or the self-seeding phenomenon. Building a general, cancer type specific, comprehensive theory that would integrate these dynamical processes remains an open challenge. On the therapeutic side, recent studies demonstrated that some drugs (such as the Sunitinib), while having a positive effect on the primary tumor (reduction of the growth), could *accelerate* the growth of the metastases. Moreover, this effect was found to be scheduling-dependent. Designing better ways to use this drug in order to control these phenomena is another challenge. In the context of combination therapies, the question of the *sequence* of administration between the two drugs is also particularly relevant.

One of the technical challenge that we need to overcome when dealing with biological data is the presence of potentially very large inter-animal (or inter-individual) variability.

Starting from the available multi-modal data and relevant biological or therapeutic questions, our purpose is to develop adapted mathematical models (*i.e.* identifiable from the data) that recapitulate the existing knowledge and reduce it to its more fundamental components, with two main purposes:

1. to generate quantitative and empirically testable predictions that allow to assess biological hypotheses or
2. to investigate the therapeutic management of the disease and assist preclinical studies of anticancerous drug development.

We believe that the feedback loop between theoretical modeling and experimental studies can help to generate new knowledge and improve our predictive abilities for clinical diagnosis, prognosis, and therapeutic decision. Let us note that the first point is in direct link with the axes 1 and 2 of the team since it allows us to experimentally validate the models at the biological scale (*in vitro* and *in vivo* experiments) for further clinical applications.
More precisely, we first base ourselves on a thorough exploration of the biological literature of the biological phenomena we want to model: growth of tumor spheroids, in vivo tumor growth in mice, initiation and development of the metastases, effect of anti-cancerous drugs. Then we investigate, using basic statistical tools, the data we dispose, which can range from: spatial distribution of heterogeneous cell population within tumor spheroids, expression of cell makers (such as green fluorescent protein for cancer cells or specific antibodies for other cell types), bioluminescence, direct volume measurement or even intra-vital images obtained with specific imaging devices. According to the data type, we further build dedicated mathematical models that are based either on PDEs (when spatial data is available, or when time evolution of a structured density can be inferred from the data, for instance for a population of tumors) or ODEs (for scalar longitudinal data). These models are confronted to the data by two principal means:

1. when possible, experimental assays can give a direct measurement of some parameters (such as the proliferation rate or the migration speed) or
2. statistical tools to infer the parameters from observables of the model.

This last point is of particular relevance to tackle the problem of the large inter-animal variability and we use adapted statistical tools such as the mixed-effects modeling framework.

Once the models are shown able to describe the data and are properly calibrated, we use them to test or simulate biological hypotheses. Based on our simulations, we then aim at proposing to our biological collaborators new experiments to confirm or infirm newly generated hypotheses, or to test different administration protocols of the drugs. For instance, in a collaboration with the team of the professor Andreas Bikfalvi (Laboratoire de l’Angiogénèse et du Micro-environnement des Cancers, Inserm, Bordeaux), based on confrontation of a mathematical model to multi-modal biological data (total number of cells in the primary and distant sites and MRI), we could demonstrate that the classical view of metastatic dissemination and development (one metastasis is born from one cell) was probably inaccurate, in mice grafted with metastatic kidney tumors. We then proposed that metastatic germs could merge or attract circulating cells. Experiments involving cells tagged with two different colors are currently performed in order to confirm or infirm this hypothesis.

Eventually, we use the large amount of temporal data generated in preclinical experiments for the effect of anti-cancerous drugs in order to design and validate mathematical formalisms translating the biological mechanisms of action of these drugs for application to clinical cases, in direct connection with the axis 1. We have a special focus on targeted therapies (designed to specifically attack the cancer cells while sparing the healthy tissue) such as the Sunitinib. This drug is indeed indicated as a first line treatment for metastatic renal cancer and we plan to conduct a translational study coupled between A. Bikfalvi’s laboratory and medical doctors, F. Cornelis (radiologist) and A. Ravaud (head of the medical oncology department).

4. Application Domains

4.1. Tumor growth monitoring and therapeutic evaluation

Each type of cancer is different and requires an adequate model. More specifically, we are currently working on the following diseases:

- Glioma (brain tumors) of various grades,
- Metastases to the lung, liver and brain from various organs,
- Soft-tissue sarcoma,
- Kidney cancer and its metastases,
- EGFR-mutated lung cancer.

In this context our application domains are

- Image-driven patient-specific simulations of tumor growth and treatments,
- Parameter estimation and data assimilation of medical images.
4.2. Biophysical therapies
- Modeling of electrochemotherapy on biological and clinical scales.
- Evaluation of radiotherapy and radiofrequency ablation.

4.3. In-vitro and animals experimentations in oncology
- Theoretical biology of the metastatic process: dynamics of a population of tumors in mutual interactions, dormancy, pre-metastatic and metastatic niche, quantification of metastatic potential and differential effects of anti-angiogenic therapies on primary tumor and metastases.
- Mathematical models for preclinical cancer research: description and prediction of tumor growth and metastatic development, effect of anti-cancerous therapies.

5. Highlights of the Year

5.1. Highlights of the Year
The team published in medical journals with strong impact factors like Cancer Research (Mathematical modeling of tumor-tumor distant interactions supports a systemic anti-proliferative control of tumor growth by S. Benzekry, et al for instance).
A new promising collaboration has started with the group of Yuval Shaked (double ERC laureate) at the Technion Israel Institute of Technology and first joint publication Dose- and time-dependence of the host-mediated response to paclitaxel therapy: a mathematical modeling approach by Benguigui et al will appear in Oncotarget, 2017.
Sébastien Benzekry received of the title of Assistant Associate Professor in the Department of Medical Biosciences of Iowa State University, reinforcing a starting collaboration with Jonathan Mochel about PK/PD modeling for comparative oncology.
Two former members of the team (Thierry Colin and Vivien Pianet) were hired by Sophia Genetics (http://www.sophiagenetics.com) to build its new imaging department and developed works initiated in Monc.

6. New Results

6.1. Mathematical modeling of tumor-tumor distant interactions supports a systemic control of tumor growth
Authors: Sébastien Benzekry, Clare Lamont, Dominique Barbolosi, Lynn Hlatky, Philip Hahnfeldt. Paper published in Cancer Research, https://hal.inria.fr/hal-01566947.
Interactions between different tumors within the same organism have major clinical implications, especially in the context of surgery and metastatic disease. Three main explanatory theories (competition, angiogenesis inhibition and proliferation inhibition) have been proposed but precise determinants of the phenomenon remain poorly understood. Here we formalized these theories into mathematical models and performed biological experiments to test them with empirical data. In syngeneic mice bearing two simultaneously implanted tumors, growth of only one of the tumors was significantly suppressed (61% size reduction at day 15, p<0.05). The competition model had to be rejected while the angiogenesis inhibition and proliferation inhibition models were able to describe the data. Additional models including a theory based on distant cytotoxic log-kill effects were unable to fit the data. The proliferation inhibition model was identifiable and minimal (4 parameters), and its descriptive power was validated against the data, including consistency in predictions of single tumor growth when no secondary tumor was present. This theory may also shed new light on single cancer growth insofar as it offers a biologically translatable picture of how local and global action may combine to control
local tumor growth, and in particular, the role of tumor-tumor inhibition. This model offers a depiction of concomitant resistance that provides an improved theoretical basis for tumor growth control and may also find utility in therapeutic planning to avoid post-surgery metastatic acceleration. Major findings In mice bearing two tumors implanted simultaneously, tumor growth was suppressed in one of the two tumors. Three theories of this phenomenon were advanced and assessed against the data. As formalized, a model of competition for nutrients was not able to explain the growth behavior as well as indirect, angiogenesis-regulated inhibition or a third model based on direct systemic inhibition. This last model offers a depiction of concomitant resistance that provides an improved theoretical basis for tumor growth control and may also find utility in therapeutic planning to avoid post-surgery metastatic acceleration.

6.2. Precision of manual two-dimensional segmentations of lung and liver metastases and its impact on tumour response assessment using RECIST 1.1

Authors: François Cornelis, Marie Martin, Olivier Saut, Xavier Buy, Michèle Kind, Jean Palussière, Thierry Colin. Paper published in European Radiology Experimental, https://hal.inria.fr/hal-01634849.

Response evaluation criteria in solid tumours (RECIST) has significant limitations in terms of variability and reproducibility, which may not be independent. The aim of the study was to evaluate the precision of manual bi-dimensional segmentation of lung, liver metastases, and to quantify the uncertainty in tumour response assessment. Methods: A total of 520 segmentations of metastases from six livers and seven lungs were independently performed by ten physicians and ten scientists on CT images, reflecting the variability encountered in clinical practice. Operators manually contoured the tumours, firstly independently according to the RECIST and secondly on a preselected slice. Diameters and areas were extracted from the segmentations. Mean standard deviations were used to build regression models and 95% confidence intervals (95% CI) were calculated for each tumor size and for limits of progressive disease (PD) and partial response (PR) derived from RECIST 1.1. Results: Thirteen aberrant segmentations (2.5%) were observed without significant differences between the physicians and scientists; only the mean area of liver tumours (p = 0.034) and mean diameter of lung tumours (p = 0.021) differed significantly. No difference was observed between the methods. Inter-observer agreement was excellent (intra-class correlation >0.90) for all variables. In liver, overlaps of the 95% CI with the 95% CI of limits of PD or PR were observed for diameters above 22.7 and 37.9 mm, respectively. An overlap of 95% CIs was systematically observed for area. No overlaps were observed in lung. Conclusions: Although the experience of readers might not affect the precision of segmentation in lung and liver, the results of manual segmentation performed for tumor response assessment remain uncertain for large liver metastases.

6.3. Dose- and time-dependence of the host-mediated response to paclitaxel therapy: a mathematical modeling approach

Authors: Madeleine Benguigui, Dror Alishkevitz, Michael Timaner, Dvir Shechter, Ziv Raviv, Sebastien Benzekry, Yuval Shaked. Paper published in OncoTarget, https://hal.inria.fr/hal-01672568.

It has recently been suggested that pro-tumorigenic host-mediated processes induced in response to chemotherapy counteract the anti-tumor activity of therapy, and thereby decrease net therapeutic outcome. Here we use experimental data to formulate a mathematical model describing the host response to different doses of paclitaxel (PTX) chemotherapy as well as the duration of the response. Three previously described host-mediated effects are used as readouts for the host response to therapy. These include the levels of circulating endothelial progenitor cells in peripheral blood and the effect of plasma derived from PTX-treated mice on migratory and invasive properties of tumor cells in vitro. A first set of mathematical models, based on basic principles of pharmacokinetics/pharmacodynamics, did not appropriately describe the dose-dependence and duration of the host response regarding the effects on invasion. We therefore provide an alternative mathematical model with a dose-dependent threshold, instead of a concentration-dependent one, that describes better the data. This model is integrated into a global model defining all three host-mediated effects. It not only precisely describes the data, but also correctly predicts host-mediated effects at different doses as well as the duration of the host
response. This mathematical model may serve as a tool to predict the host response to chemotherapy in cancer patients, and therefore may be used to design chemotherapy regimens with improved therapeutic outcome by minimizing host mediated effects.

6.4. Tumor growth model of ductal carcinoma: from in situ phase to stroma invasion

Authors: Olivier Gallinato, Thierry Colin, Olivier Saut, Clair Poignard Paper published in Journal of Theoretical Biology, https://hal.inria.fr/hal-01598837.

This paper aims at modeling breast cancer transition from the in situ stage – when the tumor is confined to the duct – to the invasive phase. Such a transition occurs thanks to the degradation of the duct membrane under the action of specific enzymes so-called matrix metallo-proteinases (MMPs). The model consists of advection–reaction equations that hold in the duct and in the surrounding tissue, in order to describe the proliferation and the necrosis of the cancer cells in each subdomain. The divergence of the velocity is given by the increase of the cell densities. Darcy law is imposed in order to close the system. The key-point of the modeling lies in the description of the transmission conditions across the duct. Nonlinear Kedem-Katchalsky transmission conditions across the membrane describe the discontinuity of the pressure as a linear function of the flux. These transmission conditions make it possible to describe the transition from the in situ stage to the invasive phase at the macroscopic level. More precisely, the membrane permeability increases with respect to the local concentration of MMPs. The cancer cells are no more confined to the duct and the tumor invades the surrounding tissue. The model is enriched by the description of nutrients concentration, tumor necrosis factors, and MMPs production. The mathematical model is implemented in a 3D C++-code, which is based on well-adapted finite difference schemes on Cartesian grid. The membrane interface is described by a level-set, and the transmission conditions are precisely approached at the second order thanks to well-suited sharp stencils. Our continuous approach provides new significant insights in the macroscopic modeling of the breast cancer phase transition, due to the membrane degradation by MMP enzymes.

6.5. Superconvergent second order Cartesian method for solving free boundary problem for invadopodia formation

Authors: Olivier Gallinato, Clair Poignard. Paper published in Journal of Computational Physics, https://hal.inria.fr/hal-01483484.

In this paper, we present a superconvergent second order Cartesian method to solve a free boundary problem with two harmonic phases coupled through the moving interface. The model recently proposed by the authors and colleagues describes the formation of cell protrusions. The moving interface is described by a level set function and is advected at the velocity given by the gradient of the inner phase. The finite differences method proposed in this paper consists of a new stabilized ghost fluid method and second order discretizations for the Laplace operator with the boundary conditions (Dirichlet, Neumann or Robin conditions). Interestingly, the method to solve the harmonic subproblems is superconvergent on two levels, in the sense that the first and second order derivatives of the numerical solutions are obtained with the second order of accuracy, similarly to the solution itself. We exhibit numerical criteria on the data accuracy to get such properties and numerical simulations corroborate these criteria. In addition to these properties, we propose an appropriate extension of the velocity of the level-set to avoid any loss of consistency, and to obtain the second order of accuracy of the complete free boundary problem. Interestingly, we highlight the transmission of the superconvergent properties for the static subproblems and their preservation by the dynamical scheme. Our method is also well suited for quasistatic Hele-Shaw-like or Muskat-like problems.

6.6. A Voronoi Interface approach to cell aggregate electropermeabilization

Authors: Arthur Guittet, Clair Poignard, Frederic Gibou.
In this work, a Voronoi Interface approach to the study of cell electropermeabilization is presented. We consider the nonlinear electropermeabilization model of Poignard et al., which takes into account the jump in the voltage potential across cells’ membrane. The jump condition is imposed in a sharp manner, using the Voronoi Interface Method of Guittet et al., while adaptive Quad-/Oc-tree grids are employed to automatically refine near the cells boundary for increased accuracy. Numerical results are provided to illustrate the accuracy of the methods. We also carry out simulations in three spatial dimensions to investigate the influence of shadowing and of the cells shape on the degree of permeabilization.

6.7. Revisiting bevacizumab + cytotoxics scheduling using mathematical modeling: proof of concept study in experimental non-small cell lung carcinoma

Authors: D.C. Imbs, R. El Cheikh, A. Boyer, J. Ciccolini, C. Mascaux, B. Lacarelle, F. Barlesi, D. Barbolosi and S. Benzekry. Paper published in CPT Pharmacometrics Syst Pharmacol, https://hal.inria.fr/hal-01624423. Concomitant administration of bevacizumab and pemetrexed-cisplatin is a common treatment for advanced nonsquamous non-small cell lung cancer (NSCLC). Vascular normalization following bevacizumab administration may transiently enhance drug delivery, suggesting improved efficacy with sequential administration. To investigate optimal scheduling, we conducted a study in NSCLC-bearing mice. First, experiments demonstrated improved efficacy when using sequential vs. concomitant scheduling of bevacizumab and chemotherapy. Combining this data with a mathematical model of tumor growth under therapy accounting for the normalization effect, we predicted an optimal delay of 2.8 days between bevacizumab and chemotherapy. This prediction was confirmed experimentally, with reduced tumor growth of 38% as compared to concomitant scheduling, and prolonged survival (74 vs. 70 days). Alternate sequencing of 8 days failed in achieving a similar increase in efficacy, thus emphasizing the utility of modeling support to identify optimal scheduling. The model could also be a useful tool in the clinic to personally tailor regimen sequences.

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

- Research contract between Roche and Monc team.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. Plan Cancer

8.1.1.1. NUMEP


8.1.1.2. Dynamo

8.1.3. Moglimaging
- Project acronym - Moglimaging: Modeling of Glioblastoma treatment-induced resistance and heterogeneity by multi-modal imaging.
- Partners -
- Duration - from Nov. 2016 to Nov 2019.
- Team participants - S. Benzekry, A. Collin, C. Poignard, O. Saut.

8.1.4. MIMOSA
- Project acronym - Plan Cancer MIMOSA (Physique, Mathématiques et Sciences de l’ingénieur appliqués au Cancer)
- Partner - ITA V, Toulouse
- Duration - from 2014 to 2017
- Coordinator - Th. Colin
- Team participants - Th. Colin, C. Poignard, O. Saut
- Title - Mathematical modeling for exploration of the impact of mechanical constraints on tumor growth

8.1.2. Systems Biology of Renal Carcinoma using a Mouse RCC model
- Title: Plan Cancer Systems Biology of Renal Carcinoma using a Mouse RCC model
- Partners : LAMC, INSERM-Univ. Bordeaux.
- Team participants: O. Saut, S. Benzekry (co-PI)
- 116.64k€

8.1.3. Transnation call: INCA/ARC
- Title: Minimally and non-invasive methods for early detection and/or progression of cancer
- Acronym: TRANSCAN
- Team participants: A. Collin, C. Poignard, O. Saut (local PI)
- Total funds: 1M150, Monc’s share 275k€.

8.1.4. Competitivity Clusters
- Labex TRAIL (http://trail.labex.u-bordeaux.fr): MOD Project Consolidation. 1 2-years post-doc position (100k€), led by A. Collin, 1 PhD funding (100k€) led by O. Saut.

8.2. European Initiatives
MONC is partner of the European Lab EBAM devoted to electroporation. C.Poignard is member of the steering committee.

8.3. International Initiatives
MONC is partner of the Japanese Core-to-Core project « Establishing networks in mathematical medicine » coordinated by T. Suzuki (Osaka University) with Vanderbilt Univ, and St Andrews Univ. Local PIs are V. Quaranta (Vanderbilt), M. Chaplain (St Andrews) and C.Poignard (MONC).
8.3.1. Inria Associate Teams Not Involved in an Inria International Labs

8.3.1.1. METAMATS

Title: Modeling ExperimenTAl MetAsTasiS

International Partner (Institution - Laboratory - Researcher):

Roswell Park Cancer Institute (United States) - Department of Cancer Genetics Department of Medicine Department of Pharmacology and Therapeutics (Graduate Program) - John Ebos

Start year: 2017

See also: http://metamats.bordeaux.inria.fr/

The aim of the METAMATS associate team is to bring together a cancer biology experimental laboratory led by John ML Ebos (Roswell Park Cancer Institute) and the inria MONC team composed of applied mathematicians. The Ebos laboratory is specialized in the study of anti-cancer therapeutics (in particular, novel biologically targeted therapeutics such as anti-angiogenics and immunotherapies) on the development of metastases and produces unique, hard-to-obtain data sets on this process’ dynamics. The MONC team is specialized in mathematical models in oncology, with a dedicated axis about modeling support and methodological development for analysis of data from preclinical studies. In particular, the work of S. Benzekry puts emphasis on proposing, studying and validating mathematical models of metastatic development under the action of various therapeutic modalities. Indeed, metastatic expansion remains the main challenge in the treatment of cancer and integrative studies combining experiments, mathematical models and clinical data have the potential to yield predictive computational tools of help to assist both the design of clinical trials and clinical oncologists in therapeutic decisions such as the control of the toxicity/efficacy balance or the optimal combination of treatment modalities.

8.3.1.2. Num4SEP

Title: Numerics for Spherical Electroporation

International Partner (Institution - Laboratory - Researcher):

University of California, Santa Barbara (United States) - ___Mechanical Engineering___ - Frederic Gibou

Start year: 2017

See also: http://num4sep.bordeaux.inria.fr/

Electroporation-based therapies (EPTs) consist in applying high voltage short pulses to cells in order to create defects in the plasma membrane. They provide interesting alternatives to standard ablative techniques, for instance for deep seated badly located tumors. However their use is still limited due to a lack of knowledge of tissue electroporation. The goal of the associate team is to focus on the multiscale numerical modeling of spheroid electroporation, in order to provide new insights in electroporation at the mesoscopic scales (spheroids provide interesting tumor-like biological models). Benefiting from the expertise of F. Gibou’s team in HPC for multiphysics, and the expertise of the team MONC in tumor growth and cell electroporation modeling, the goal of the associate team Num4SEP is to obtain accurate and efficient numerical tools for the quantitative evaluation of the EPTs at the mesoscopic scale.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Selection

9.1.1.1. Member of the Conference Program Committees
- Sébastien Benzekry: Membre du comité scientifique des Mathematical Biology Modeling days of Besançon, MB² (http://mb2.univ-fcomte.fr/index.html).
- Clair Poignard: Organisation of the Theoretical Physics Day at the University of Bordeaux.

### 9.1.2. Journal

#### 9.1.2.1. Member of the Editorial Boards
- Sébastien Benzekry: Invited editor of a special issue of the journal Complexity : "Mathematical Oncology: Unveiling Biological Complexity Using Mathematical Methods"
- Clair Poignard: Member of the editorial committee of DCDS-S.

#### 9.1.2.2. Reviewer - Reviewing Activities
- Olivier Saut : PLOS One, Nature Comm, Medical Image Analysis.

### 9.1.3. Invited Talks
- Clair Poignard: Conference in honor of the 60th Birthday of Y. Maday. Electroporation modeling, from cell to tissue.

### 9.1.4. Scientific Expertise
- Sébastien Benzekry: Reviewer for the Foundation for Polish Science (TEAM programme), European funds Smart Growth
- Clair Poignard: Member of the evaluation committee of the call of the Plan Cancer «Physique pour le Cancer »
- Olivier Saut: O. Saut is an expert for the French Ministry of Research (for various programs including PHC and EGIDE programs).
- Olivier Saut: reviewer for IDEX Université Grenoble Alpes projects.
9.1.5. Research Administration

- Clair Poignard: Member of the Inria evaluation committee.
- Olivier Saut: member of the steering committee of Labex TRAIL (Translational Imaging) http://trail.labex.u-bordeaux.fr.
- Olivier Saut: member of the steering committee of ITMO consortium HTE (on tumor heterogeneity) and coordinator of work package Model and Data.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence: S. Benzekry, Analyse numérique, 24h ETD, L3, Bordeaux INP, France
Licence : A. Collin, TD EDO, 48h, niveau L3, INP Bordeaux, France.
Master : A. Collin, TP C++, 96h, niveau M1, INP Bordeaux, France.
Master : A. Collin, Cours de maillage, 36h, niveau M2, INP Bordeaux, France.
Master : A. Collin, Encadrement de projets, 30h, niveaux M1, M2, INP Bordeaux, France.
Licence : C. Poignard, Undergraduate teaching in Numerical and Applied Mathematics (L3, M1) 80heqTD: IPB, ENSAM.

9.2.2. Supervision

- PhD: Manon Deville, Mathematical Modeling of enhanced drug delivery by mean of Electroporation or Enzymatic treatment, University of Bordeaux (cotutelle with R. Natalini, University of Rome Tor Vergata), 22 November 2017, Clair Poignard.
- PhD: Agathe Peretti, Quantification de l’hétérogénéité tumorale à partir de l’imagerie médicale. Application à la classification de tumeurs rénales, Université de Bordeaux, 20 décembre 2017, Thierry Colin, Olivier Saut.
- PhD in progress: T. Kritter, Primary tumors modeling with a view to the gliomas and adenocarcinomas study, Sep 2015, C. Poignard and O. Saut
- PhD in progress: S. Corridore, Mathematical Model for Electroporation, A. Collin, C. Poignard.
- PhD in progress: C. Perier, 2016-2019, B. Denis de Senneville and O. Saut, Combining texture analysis and modeling for evaluation therapies and clinical outcome.
- PhD in progress: A. Crombé, 2017-2020, O. Saut, Beyond radiomics for soft-tissue sarcoma.

9.2.3. Juries

- Sébastien Benzekry: Committee member of the PhD thesis of K. El Alaoui Lasmaili, Université de Lorraine (mention Sciences de la Vie et de la Santé), 4 Avril 2017.
- Clair Poignard: reviewer of the PhD thesis of A. Barlukova (Université Aix-Marseille),
- Clair Poignard: reviewer of the PhD thesis of K. Van Nguyen (Ecole Polytechnique X)
- Clair Poignard: Committee member of the PhD thesis of T. Wintz: Super-resolution in wave imaging. (ENS Paris)
9.3. Popularization

- Sébastien Benzekry: Interview for the journal « Sciences et Avenir ».
- A. Collin : Printemps de la mixité (a presentation on scientific calculation in front of 2 classes of the first year), Institut Mathématiques de Bordeaux, 04/04/17, https://www.u-bordeaux.fr/Actualites/De-l-universite/Le-Printemps-de-la-mixite.
- A. Collin: Cinéma Sciences (discussion with the public on mathematics after the projection of the film "Les figures de l’ombre"), Cinéma de Mérignac 18/05/2017.

10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


bevacizumab + paclitaxel doublet leads to reduced tumor growth and fewer metastasis, in "Oncotarget", 2017 [DOI : 10.18632/oncotarget.15484], https://hal.inria.fr/hal-01474679.


International Conferences with Proceedings

National Conferences with Proceeding


Scientific Books (or Scientific Book chapters)


Research Reports

Project-Team PHOENIX

Programming Language Technology
For Communication Services

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed programming and Software engineering
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10. Bibliography
Project-Team PHOENIX

Creation of the Project-Team: 2005 September 08, end of the Project-Team: 2017 December 31

Keywords:

**Computer Science and Digital Science:**
- A1.2.5. - Internet of things
- A1.4. - Ubiquitous Systems
- A2.1. - Programming Languages
- A2.4.2. - Model-checking
- A2.5. - Software engineering
- A2.6.2. - Middleware
- A5.1. - Human-Computer Interaction
- A5.11. - Smart spaces

**Other Research Topics and Application Domains:**
- B1.2.2. - Cognitive science
- B2.1. - Well being
- B2.5.2. - Cognitive disabilities
- B2.5.3. - Assistance for elderly
- B4.5. - Energy consumption
- B8. - Smart Cities and Territories

1. Personnel

**Research Scientists**
- Bernard Serpette [Inria, Researcher, from Mar 2017]
- Eugene Volanschi [Inria, Advanced Research Position]

**Faculty Members**
- Charles Consel [Team leader, Institut National Polytechnique de Bordeaux, Professor, HDR]
- Helene Sauzeon [Univ de Bordeaux, Professor, HDR]

**External Collaborator**
- Bernard N Kaoua [Univ de Bordeaux]

**Technical Staff**
- Quentin Barlas [Inria]
- Julien Durand [Inria, until Oct 2017]
- Leo Mendiboure [Inria, from Oct 2017]
- Ludovic Fornasari [Inria, Engineers]
- Amandine Desrozier [Inria, Research technician]
- Pauline Fontagne [Inria, Research technician, until October 2017]
- Flora Gallet [Inria, Research technician]

**PhD Students**
- Rafik Belloum [Inria]
- Adrien Carteron [Inria]
- Audrey Landuran [Univ de Bordeaux]
- Cécile Mazon [Inria]
2. Overall Objectives

2.1. Context

A host of networked entities (devices and services) are populating smart spaces that become prevalent (e.g., building management, personal assistance, avionics) and large scale (e.g., train station, city, highway network). These smart spaces are becoming intimately intertwined with our daily life and professional activities, raising scientific challenges that go beyond the boundaries of single field of expertise.

2.2. A Multi-Disciplinary Approach

We focus our attention on the domain of applications that orchestrate networked objects, whether populating smart spaces or worn by individuals on-the-go. Because such applications are intimately intertwined with the users’ daily life and professional activities, they can improve users’ efficiency in performing tasks or compensate for the users’ deficiencies and disabilities, promoting autonomy. However, this emerging domain of assistive computing raises scientific challenges that go beyond the boundaries of Computer Science. To address these challenges, the Phoenix group has been conducting interdisciplinary research that combines

- Cognitive Science to study user needs and make a rigorous assessment of the services provided to users;
- Sensing and actuating expertise to support users, based on accurate and rich interactions with their environment;
- Design-driven software engineering to support and guide all the development process of the services provided to users.

2.3. Research Avenues

The activities of the Phoenix group revolve around three main avenues of research.

Design-driven software development. We further the study of design-driven software development, exploring the integration of both functional and non-functional concerns in the design phase, as well as the human-computer interaction dimension. We also expand the scope of our approach by scaling it up to the orchestration of masses of sensors and actuators.

Assistive computing in the home. This line of work leverages DiaSuite to develop an assisted living platform, named HomeAssist, which exploits the capabilities of smart spaces to provide services that compensate or remediate cognitive difficulties of users, drawn from needs analyses. This work is validated in the context of two research projects: HomeAssist for older adults, and ANDDI for adults with Intellectual Disabilities (ID). This platform is currently deployed in the homes of older adults where a variety of applications assist them with their daily activities.

Assistive computing on-the-go. We develop mobile assistive computing support based on tablets. In particular, we have developed a cognitive assistive technology for the inclusion of children with Autism in mainstreamed environments, named School+. 
3. Research Program

3.1. Design-Driven Software Development

Raising the level of abstraction beyond programming is a very active research topic involving a range of areas, including software engineering, programming languages and formal verification. The challenge is to allow design dimensions of a software system, both functional and non-functional, to be expressed in a high-level way, instead of being encoded with a programming language. Such design dimensions can then be leveraged to verify conformance properties and to generate programming support.

Our research on this topic is to take up this challenge with an approach inspired by programming languages, introducing a full-fledged language for designing software systems and processing design descriptions both for verification and code generation purposes. Our approach is also DSL-inspired in that it defines a conceptual framework to guide software development. Lastly, to make our approach practical to software developers, we introduce a methodology and a suite of tools covering the development life-cycle.

To raise the level of abstraction beyond programming, the key approaches are model-driven engineering and architecture description languages. A number of architecture description languages have been proposed; they are either (1) coupled with a programming language (e.g., [25]), providing some level of abstraction above programming, or (2) integrated into a programming language (e.g., [21], [26]), mixing levels of abstraction. Furthermore, these approaches poorly leverage architecture descriptions to support programming, they are crudely integrated into existing development environments, or they are solely used for verification purposes. Model-driven software development is another actively researched area. This approach often lacks code generation and verification support. Finally, most (if not all) approaches related to our research goal are general purpose; their universal nature provides little, if any, guidance to design a software system. This situation is a major impediment to both reasoning about a design artifact and generating programming support.

3.2. Integrating Non-Functional Concerns into Software Design

Most existing design approaches do not address non-functional concerns. When they do, they do not provide an approach to non-functional concerns that covers the entire development life-cycle. Furthermore, they usually are general purpose, impeding the use of non-functional declarations for verification and code generation. For example, the Architecture Analysis & Design Language (AADL) is a standard dedicated to real-time embedded systems [22]. AADL provides language constructs for the specification of software systems (e.g., component, port) and their deployment on execution platforms (e.g., thread, process, memory). Using AADL, designers specify non-functional aspects by adding properties on language constructs (e.g., the period of a thread) or using language extensions such as the Error Model Annex. The software design concepts of AADL are still rather general purpose and give little guidance to the designer.

Beyond offering a conceptual framework, our language-based approach provides an ideal setting to address non-functional properties (e.g., performance, reliability, security, ...). Specifically, a design language can be enriched with non-functional declarations to pursue three goals: (1) expanding further the type of conformance that can be checked between the design of a software system and its implementation or execution infrastructure, (2) enabling additional programming support and guidance, and (3) leveraging the design declarations to optimize the generated implementation.

We are investigating this idea by extending our design language with non-functional declarations. For example, we have addressed error handling [9], access conflicts to resources [24], quality of service constraints [23], and more recently, data delivery models and parallel computation models for masses of sensors [14].

Following our approach to paradigm-oriented software development, non-functional declarations are verified at design time, they generate support that guides and constrains programming, they produce a runtime system that preserves invariants and performs efficiently.

The Error Model Annex is a standardized AADL extension for the description of errors [27].
3.3. Human-Driven Software Design

Knowledge of the human characteristics (individual, social and organizational) allow the design of complex system and artifacts for increasing their efficacy. In our approach of assistive computing, a main challenge is the integration of facets of Human Factors in order to design technology support adapted to user needs in term of ergonomic properties (acceptability, usability, utility etc) and delivered functionalities (oriented task under user abilities contraints).

We adapt this approach to improve the independent living and self-determination of users with cognitive impairments by developing a variety of orchestration scenarios of networked objects (hardware/software) to provide a pervasive support to their activities. Human factors methodologies are adopted in our approach with as direct purpose the reliability and efficiency of the performance of digital support systems in respect of objectives of health and well-being of the person (monitoring, evaluation, and rehabilitation).

Precisely, our methodologies are based on a closed iterative loop, as described in the figure below :

- Identifying the person needs in a natural situation (i.e., desired but problemactic activities) according to Human Factors Models of activity (i.e., environmental constraints; social support networks - caregivers and family; person’s abilities)
- Designing environmental support that will assist the users to bypass their cognitive impairment (according to environmental models of cognitive compensatory mechanisms); and then implement this support in terms of technological solutions (scenarios of networked objects, hardware interface, software interface, interaction style, etc)
- Empirically evaluating the assistive solution based on human experimentations that includes ergonomic assessments (acceptability, usability, usefulness, etc) as well as longitudinal evaluations of use’s efficacy in terms of activities performed by the individual, of satisfaction and well-being provided to the individual but also to his/her entourage (family and caregivers).

4. Application Domains

4.1. Internet of Things

Participants: Charles Consel, Nic Volanschi.

The Internet of Things (IoT) has become a reality with the emergence of Smart Cities, populated with large amounts of smart objects which are used to deliver a range of citizen services (e.g., security, well being, etc.) The IoT paradigm relies on the pervasive presence of smart objects or “things”, which raises a number of new challenges in the software engineering domain.

We introduce a design-driven development approach that is dedicated to the domain of orchestration of masses of sensors. The developer declares what an application does using a domain-specific language (DSL), named DiaSwarm. Our compiler processes domain-specific declarations to generate a customized programming framework that guides and supports the programming phase.

DiaSwarm addresses the main phases of an application orchestrating masses of sensors.

Service discovery  Standard service discovery at the individual object level does not address the needs of applications orchestrating large numbers of smart objects. Instead, a high-level approach which provides constructs to specifying subsets of interest is needed. Our approach allows developers to introduce application-specific concepts (e.g., regrouping parking spaces into lots or districts) at the design time and then these can be used to express discovery operations. Following our design-driven development approach, these concepts are used to generate code to support and guide the programming phase.
Figure 1. User-Centered Approach
Data gathering  Applications need to acquire data from a large number of objects through a variety of delivery models. For instance, air pollution sensors across a city may only push data to the relevant applications when pollution levels exceed tolerated levels. Tracking sensors, however, might determine the location of vehicles and send the acquired measurements to applications periodically (e.g., 10 min. intervals). Data delivery models need to be introduced at design time since they have a direct impact on the application’s program structure. In doing so, the delivery models used by an application can be checked against sensor features early in the development process.

Data processing  Data that is generated from hundreds of thousands of objects and accumulated over a period of time calls for efficient processing strategies to ensure the required performance is attained. Our approach allows for an efficient implementation of the data processing stage by providing the developer with a framework based on the MapReduce [34] programming model which is intended for the processing of large data sets.

4.2. Assistive computing in the home


In this avenue of research, we have been developing a systemic approach to introducing an assisted living platform for the home of older adults. To do so, we formed an interdisciplinary team that allows (1) to identify the user needs from a gerontological and psychological viewpoint; (2) to propose assistive applications designed by human factors and HCI experts, in collaboration with caregivers and users; (3) to develop and test applications designed and developed by software engineers; (4) to conduct a field study to assess the benefits of the platform and assistive applications, in collaboration with caregivers, by deploying the system at the actual homes.

Our research activities for assistive computing in the home are conducted under the HomeAssist project. This work takes the form of a platform offering an online catalog of assistive applications that orchestrate an open-ended set of networked objects. Our platform leverages DiaSuite to quickly and safely develop applications at a high level.

Our scientific achievements include the design principles of our platform, its key features to effectively assist individuals in their home, field studies to validate HomeAssist, the expansion of HomeAssist to serve individuals with ID, and the technology transfer of HomeAssist. Note that a complete presentation of this work, from a Cognitive Science perspective, is given in the doctoral thesis of Lucile Dupuy published last year (2016).

4.2.1. Project-team positioning

There is a range of platforms for assisted living aimed at older adults that have been developed for more than a decade. Most of these platforms are used in a setting where participants come to a research apartment to perform certain tasks. This setting makes it difficult to assess user acceptance and satisfaction of the proposed approaches because the user does not interact with the technology on a daily basis, over a period of time. Furthermore, older adults adopt routines to optimize their daily functioning at home. This situation calls for field studies in a naturalistic setting to strengthen the evaluation of assisted living platforms.

HomeAssist innovates in that it supports independent living across the activities of daily living and is validated by field studies in naturalistic setting.

4.3. Assistive computing on-the-go

Participants: Cécile Mazon, Léo Mendiboure, Hélène Sauzéon, Charles Consel.

We conduct research on assistive computing supported by mobile devices such as smart phones and tablets. Both research projects presented in this section are supported by tablets and leverage their functionalities
to guide users with cognitive challenges performing activities and tasks, whether in mainstream schools to support inclusion or in residential settings to support their autonomy. The mobile nature of tablets allows to envision such devices as supporting users with cognitive challenges across a range of environments.

Many research projects bring cognitive-support applications to users based on tablets and smartphones. However, few projects equip users with such devices in actual mainstream environments, including stakeholders in the design process and targeting an autonomous usage of assistive applications. An additional originality of our approach is our interdisciplinary approach that allows us to integrate key psychological dimensions in our design, such as self-determination.

4.4. Life Plan

Participants: Audrey Landuran, Gregory Lecouvey, Léo Mendiboure, Quentin Barlas, Bernard N’Kaoua.

Elaboration of life plan is a major stage in the developmental trajectory of people with intellectual deficiency and is based on several capabilities: make choices, express them, be aware of their consequences, etc. However, these various capabilities can raise problems for people with Down syndrome. The aim of this project has been to design and validate a digital assistant that allows to help the individuals to make choices, to plan for the future and to define their life plan. The user-centered methodology employed has allowed to involve the people with Down syndrome, their families and their caregivers in all stages of design. Different validations achieved attest for the accessible, friendly, funny character of the assistant and its ability to promote the expression of the life plan in accordance with individuals’ choices, wishes and desires.

The digital assistant is now available online at: http://www.monprojetdevie.trisomie21-france.org/.

5. Highlights of the Year

5.1. Highlights of the Year

The College+ software, an assistive application on iPad for children with Autism Spectrum Disorders included in ordinary schools, has been distributed on the Apple store, starting in October 2017.


6. New Software and Platforms

6.1. College

KEYWORDS: Neurosciences - Health - Autism - Mobile application

FUNCTIONAL DESCRIPTION: College+ is an iPad app gathering an assistance module and a training module for school inclusion in of children with autism spectrum disorders and children with intellectual disabilities in mainstream classrooms. The assistance module, used in mainstream classroom, comprises 3 functionalities: - emotion regulation - classroom routines - verbal communication. The training module, used on a daily basis at home or in special education classroom, comprises two functionalities, presented as serious games: - attention training - emotion identification training. All contents of College+ app can be modified, to fit the unique needs of each student.

- Participants: Alexandre Spriet, Charles Consel, Charles Fage, Damien Martin Guillerez and Hélène Sauzéon
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Charles Consel
- URL: http://phoenix.inria.fr/research-projects/school
Figure 2. Sample screenshots from the Life Plan website.
6.2. College +

**KEYWORDS**: Neurosciences - Health - Autism - Mobile application

**FUNCTIONAL DESCRIPTION**: College+ is an iPad app gathering an assistance module and a training module for school inclusion in of children with autism spectrum disorders and children with intellectual disabilities in mainstream classrooms. The assistance module, used in mainstream classroom, comprises 3 functionalities: - emotion regulation - classroom routines - verbal communication. The training module, used on a daily basis at home or in special education classroom, comprises two functionalities, presented as serious games: - attention training - emotion identification training. All contents of College+ app can be modified, to fit the unique needs of each student.

- **Participants**: Alexandre Spriet, Charles Fage, Damien Martin Guillerez and Hélène Sauzéon
- **Contact**: Charles Consel
- **URL**: http://phoenix.inria.fr/research-projects/school

6.3. DiaSuite

**KEYWORDS**: Pervasive computing - Code generation - Specification language

**SCIENTIFIC DESCRIPTION**: DiaSuite is a suite of tools covering the development life-cycle of a pervasive computing application:

- **Defining an application area**: First, an expert defines a catalog of entities, whether hardware or software, that are specific to a target area. These entities serve as building blocks to develop applications in this area. They are gathered in a taxonomy definition, written in the taxonomy layer of the DiaSpec language.

- **Designing an application**: Given a taxonomy, the architect can design and structure applications. To do so, the DiaSpec language provides an application design layer. This layer is dedicated to an architectural pattern commonly used in the pervasive computing domain. Describing the architecture application allows to further model a pervasive computing system, making explicit its functional decomposition.

- **Implementing an application**: We leverage the taxonomy definition and the architecture description to provide dedicated support to both the entity and the application developers. This support takes the form of a Java programming framework, generated by the DiaGen compiler. The generated programming framework precisely guides the developer with respect to the taxonomy definition and the architecture description. It consists of high-level operations to discover entities and interact with both entities and application components. In doing so, it abstracts away from the underlying distributed technologies, providing further separation of concerns.

- **Testing an application**: DiaGen generates a simulation support to test pervasive computing applications before their actual deployment. An application is simulated in the DiaSim tool, without requiring any code modification. DiaSim provides an editor to define simulation scenarios and a 2D-renderer to monitor the simulated application. Furthermore, simulated and actual entities can be mixed. This hybrid simulation enables an application to migrate incrementally to an actual environment.

- **Deploying a system**: Finally, the system administrator deploys the pervasive computing system. To this end, a distributed systems technology is selected. We have developed a back-end that currently targets the following technologies: Web Services, RMI, SIP and OSGI. This targeting is transparent for the application code. The variety of these target technologies demonstrates that our development approach separates concerns into well-defined layers.
**Functional Description:** DiaSuite is developed as a research project by the Inria/LaBRI Phoenix research group. The DiaSuite approach covers the development life-cycle of a pervasive computing application. It takes the form of a methodology, supported by (1) a high-level design language and (2) a suite of tools covering the development life-cycle of a pervasive computing application. Specifically, we have developed a design language dedicated to describing pervasive computing systems and a suite of tools providing customized support for each development stage of a pervasive computing system, namely, implementation (e.g., programming support), testing (e.g., unit test, 2D simulator), and deployment (e.g., distribution platforms like SIP and Web Services).

- **Participants:** Adrien Carteron, Alexandre Spriet, Charles Consel, Milan Kabac, Paul Van Der Walt and Quentin Barlas
- **Contact:** Charles Consel
- **URL:** [http://phoenix.inria.fr/software/diasuite](http://phoenix.inria.fr/software/diasuite)

### 6.4. DiaSuiteBOX

**Keywords:** Dedicated langage - Iot - Orchestration - Toolbox - Development tool suite

**Functional Description:** DiaSuiteBOX proposes an application store that gathers the devices deployed at home. This store is open and available online such as an application store for Smartphone.

- **Participants:** Adrien Carteron, Amélie Marzin, Bertran Benjamin, Bruneau Julien, Consel Charles, Damien Cassou, Damien Martin Guillerez, Emilie Balland, Eugène Volanschi, Hélène Sauzéon, Joan Rieu, Julien Durand, Ludovic Formasari, Milan Kabac, Quentin Barlas and Quentin Enard
- **Contact:** Charles Consel
- **URL:** [https://domassist.bordeaux.inria.fr/](https://domassist.bordeaux.inria.fr/)

### 6.5. DomAssist

**Keywords:** Health - Mobile application - Persons attendant - Home care

**Functional Description:** 3 mobile applications for assistive living:
- **DiAndroid**: Interface for the main tablet with the DiaSuiteBox applications including those for the daily activities, the meetings scheduling, etc. and for home and personal safety
- **Accueil**: home screen restraining the use of a secondary tablet and offering communications and social activities applications with simplified communication means (ie. eMail), collaborative games, etc.
- **eMail**: mail client made for older people

Other Vera gateway tools:
- **Controlling connected objects to the Vera home automation gateway from Android**
- **Vera push plugin to domassist cloud**: vera plugin to communicate sensor information associated with the gateway directly to DomAssist servers
- **Vera HeartBeat Plugin**: Regular sending of a frame to know that the gateway is still online

- **Participants:** Alexandre Spriet, Quentin Barlas, Charles Consel, Hélène Sauzéon and Julien Durand
- **Partners:** Université de Bordeaux - CNRS - IPB
- **Contact:** Charles Consel
- **URL:** [http://phoenix.inria.fr/research-projects/homeassist](http://phoenix.inria.fr/research-projects/homeassist)
7. New Results

7.1. Everyday Functioning Benefits from an Assisted Living Platform amongst Frail Older Adults and Their Caregivers

Ambient assisted living technologies (AAL) are regarded as a promising solution to support aging in place. Yet, their efficacy has to be demonstrated in terms of benefits for independent living and for work conditions of caregivers. Hence, the purpose of this study was to assess the benefits of a multi-task AAL platform for both Frail older Individuals (FIs) and professional caregivers with respect to everyday functioning and caregiver burden. In this context, a 6-month field study involved 32 FIs living at home (half of them were equipped by the platform and the remaining half were not, as a control condition) and their caregivers. Everyday functioning measures were reported by frail participants and caregivers. Self-reported burden measures of caregiver were also collected. The main results showed that the caregiver’s estimates of everyday functioning of equipped participants were unchanged across time, while they decreased for the control participants. Also, a reduction of self-reported objective burden was obtained after 6 months of AAL intervention for the equipped group, compared to the control group. Overall, these results highlighted the potential of AAL as a relevant environmental support for preventing both functional losses in FIs and objective burden professional caregiver.

7.2. Designing Parallel Data Processing for Enabling Large-Scale Sensor Applications

Masses of sensors are being deployed at the scale of cities to manage parking spaces, transportation infrastructures to monitor traffic, and campuses of buildings to reduce energy consumption. These large-scale infrastructures become a reality for citizens via applications that orchestrate sensors to deliver high-value, innovative services. These applications critically rely on the processing of large amounts of data to analyze situations, inform users, and control devices. This work proposes a design-driven approach to developing orchestrating applications for masses of sensors that integrates parallel processing of large amounts of data. Specifically, an application design exposes declarations that are used to generate a programming framework based on the MapReduce programming model. We have developed a prototype of our approach, using Apache Hadoop. We applied it to a case study and obtained significant speedups by parallelizing computations over twelve nodes. In doing so, we demonstrate that our design-driven approach allows to abstract over implementation details, while exposing architectural properties used to generate high-performance code for processing large datasets. Furthermore, we show that this high-performance support enables new, personalized services in a smart city. Finally, we discuss the expressiveness of our design language, identify some limitations, and present language extensions.

7.3. Internet of Things: From Small-to Large-Scale Orchestration

The domain of Internet of Things (IoT) is rapidly expanding beyond research, and becoming a major industrial market with such stakeholders as major manufacturers of chips and connected entities (i.e., things), and fast-growing operators of wide-area networks. Importantly, this emerging domain is driven by applications that leverage an IoT infrastructure to provide users with innovative, high-value services. IoT infrastructures range from small scale (e.g., homes and personal health) to large scale (e.g., cities and transportation systems). In this work, we argue that there is a continuum between orchestrating connected entities in the small and in the large. We propose a unified approach to application development, which covers this spectrum. To do so, we examine the requirements for orchestrating connected entities and address them with domain-specific design concepts. We then show how to map these design concepts into dedicated programming patterns and runtime mechanisms. Our work revolves around domain-specific concepts and notations, integrated into a tool-based design methodology and dedicated to develop IoT applications. We have applied our work across a spectrum of infrastructure sizes, ranging from an automated pilot in avionics, to an assisted living platform for the home of seniors, to a parking management system in a smart city.
7.4. Designing an Accessible and Engaging Email Application for Aging in Place

Supporting independent everyday functioning of older adults is a major challenge for aging in place. In particular, communication and social activities need support to prevent social isolation, cognitive and psychosocial well-being decline, and a risk of depression. This paper focuses on how technology can bring social support to isolated older-old adults (over 75 years old) and allow them to communicate with members of their social network. We present the design of an accessible and engaging email application dedicated to this population. We propose design principles based on the older adults’ specificities and then use these principles to develop a tablet-based email application. We conducted a field study to evaluate our email application during 9 months. We equipped 13 community-dwelling old-older adults with a touchscreen tablet and our application at their home (compared to 13 control counterparts). This field study validates our design principles as shown by the effectiveness and efficiency gained by the participants in using our application. Moreover, we reveal the influence of health indicators in the usage behaviors and the long-term use of our application.

7.5. HomeAssist: An Assisted Living Platform for Aging in Place Based on an Interdisciplinary Approach

HomeAssist is an assisted living platform aims to support aging in place. This platform was designed using a human-centered approach. It offers assistive services, addressing the main aspects of daily life: activities of daily living, home and user safety, and social participation. HomeAssist introduces key novel features: (1) it covers multiple aspects of daily life, addressing a variety of needs of older adults; (2) it provides customization mechanisms, adapting assistance to the user’s abilities while preventing autonomy losses; (3) it relies on context awareness, delivering timely assistance; and, (4) it revolves around a unified user interface to achieve usability. All these features play a key role towards achieving high acceptance of HomeAssist and supporting autonomy effectively, as shown by our field study.

8. Partnerships and Cooperations

8.1. Regional Initiatives


ANDDI leverages the abilities of individuals with ID and the recent technological advances to develop a variety of assistive services addressing their daily needs. These services draw on our expertise in cognitive science and computer science, dedicated to assisting users with technologies. In particular, we use our platform, named HomeAssist, dedicated to the independently living of older adults. This project is funded by the Region of Aquitaine.


We conduct a Randomized Controlled Trial (RCT) of HomeAssist with older adults, ranging from autonomous to mildly cognitively impaired (e.g., Alzheimer disease (AD) in its early stage). The RCT is considered as the gold standard of a true experimental design. Furthermore, it provides strong evidence for causal relationships, as well as the ability to generalize the results to people outside the study’s sample. The study design will thus be a single-blinded RCT. It will include up to 500 participants, matched with non-equipped participants. The HomeAssist intervention will involve monitoring as well as compensation services to support independent living in place. The duration of the HomeAssist intervention is of 12 months. This project is funded by the Region of Aquitaine, the Districts of Gironde and Pyrénées Atlantique, CARSAT Aquitaine, UDCCAS, and CNSA.
8.2. National Initiatives

8.2.1. School Inclusion for Children with Autism

The objective of this project is to provide children with assistive technologies dedicated to the school routines. This project is in collaboration with the “Handicap et Système Nerveux” research group (EA 4136, Bordeaux University), the PsyCLÉ research center (EA 3273, Provence Aix-Marseille University) and the “Parole et Langage” research laboratory (CNRS, Provence Aix-Marseille University).

This work is funded by the French Ministry of National Education and Orange Foundation.

8.3. International Initiatives

8.3.1. Participation in Other International Programs

- International exchange program Idex (2016-17) — “Memory, aging, Parkinson disease, and Virtual Reality”, with Pr. Luc Noreau, Centre Interdisciplinaire de Recherche en réadaptation et intégration sociale-University of Laval, Canada. Coordinated by P. Dehail.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. Member of the Organizing Committees

Hélène Sauzéon & Bernard N’Kaoua, in cooperation with E. Morales & B. JMcFadyen, co-organized the Summer school 2017 of Alliance Bordeaux-Laval: “Mobility in urban environment: a systemic approach centered on the person and his/her environment”, 3-5 July 2017 at University of Laval (Québec, Canada).

9.1.2. Scientific Events Selection

9.1.2.1. Member of the Conference Program Committees

Charles Consel was member of the following Program Committees:

- ICSE 2018 SEIS Track (Software Engineering in Society)
- 3rd IEEE International Conference on Collaboration and Internet Computing
- International Workshop on Pervasive Systems Integration (PerSysT 2018)
- 2018 IEEE International Conference on Cloud Computing (CLOUD 2018)

9.1.2.2. Reviewer


9.1.3. Journal

9.1.3.1. Reviewer - Reviewing Activities

9.1.4. Invited Talks

Charles Consel was invited to give talks in the following contexts:

- University of Reading
- University of Toronto
- University of Illinois at Urbana-Champaign
- University of Indiana
- Digital Silver Forum on November 28 in Helsinki.

9.1.5. Scientific Expertise

Hélène Sauzéon participated as a scientific expert for:

- National call for proposals: IRSEP call “Autism and Technology”, 2017
- Recruiting committees for:
  - Lecturer on Psychology et Ergonomics, Toulouse 2 University, 2017
  - Young researchers, Inria Bordeaux, since 2015
- The scientific committee of “Expertise center Calyxis for domestic risks” (Niort, France), working on R&D of technologies for preventing everyday accidents, thru collaboration programs between public labs and private companies.

9.1.6. Research Administration

Hélène Sauzéon has been a member of the Committee launching a new institute of advanced studies at the University of Bordeaux since 2016. In this context she participated at the design of this institute, leveraging his expertise in cognitive sciences and interdisciplinary research at Inria Bordeaux. Indeed, the aim of the institute is fostering interdisciplinary research, innovation, and creativity, by providing adequate financial support, educative and participative resources to researchers on the Bordeaux campus.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

- Master (M2) : Charles Consel, “Advanced topics — Technology surveys”, 17h, Bordeaux INP, France
- Master (M2): Hélène Sauzéon, “Handicap and assistive technology, Human factors and reliability of complex systems”, 30h, University of Bordeaux, France.
- Master (M2) : Nic Volanschi, “Advanced topics — Technology surveys”, 17h, Bordeaux INP, France
- Licence (L3) : Nic Volanschi, “Introduction to imperative programming”, 24h, Bordeaux INP, France
• Master (M2) : Antoine Riché, "Software Engineering for Smart Spaces", 8h, Bordeaux INP, France
• Licence (L3) : Cécile Mazon, “Outils pour les enfants avec troubles cognitifs et apports de la psychologie cognitive”, 6h, École d’Ergothérapie, CHU Bordeaux, France
• Licence (L3) : Cécile Mazon, “École inclusive et Technologies Numériques : Quels solutions pour les enfants avec troubles cognitifs ?”, 8h, École d’Ergothérapie, CHU Bordeaux, France
• Licence (L2) : Cécile Mazon, “Handicap cognitif et Technologies d’assistance à la vie quotidienne”, 8h, École d’Ergothérapie, CHU Bordeaux, France
• Licence (L2) : Bernard Serpette, “Functional Programming”, 35h, Université de Bordeaux, France.

E-learning
MOOC: Hélène Sauzéon and Pascal Guitton, “Digital Accessibility”, open for unrestricted attendance, on the FUN national platform, supported by the Inria Learning Lab:
• 1st session in november 2016: about 3800 registered students from 60 different countries
• 2nd session in june 2017: about 1900 registered students
The MOOC contents is still currently available on “Canal U”.

9.2.2. Supervision
PhD : Adrien Carteron, “An event-based approach to the development of home assistance services for various stakeholders”, University of Bordeaux, defended on December 22nd, 2017, co-directed by Charles Consel and Nic Volanschi.
PhD in progress : Cécile Mazon, “Personalization and evaluation of a digital assistant for school inclusion of college students with autism and/or intellectual disability”, University of Bordeaux, started in September 2016, co-directed by Hélène Sauzéon and Charles Consel.
PhD in progress: Antoine Riché, “Architectures of assistive services based on software sensors”, started in October 2016, directed by Charles Consel.
PhD in progress: Rafik Belloum, “A methodology for developing assistive services”, started in 2016, directed by Charles Consel.
PhD in progress: P.A. Cinquin, “Conception et validation d’un lecteur accessible aux personnes avec troubles cognitifs pour un système d’enseignement numérique”, started in 2016, co-directed by Hélène Sauzéon and Pascal Guitton.

9.2.3. Juries
Charles Consel was member of the thesis committee for Tizneem Jiancaro, for her thesis entitled “Technology, Design and Dementia: Design approaches, implications and considerations for an emerging field”. Supervisor: Alex Mihailidis, Ph.D P.Eng. Scientific Director AGE-WELL Network of Centres of Excellence, University of Toronto.
Hélène Sauzéon was member of the thesis committee for Castor Naomie, who performed her PhD in the Lab CHART-LUTIN (Paris 8 University).
Charles Consel and Nic Volanschi were members of the thesis committee for Adrien Carteron (as co-supervisors), for his thesis in Computer Science called “An event-based approach to the development of home assistance services for various stakeholders”, University of Bordeaux, on December 22nd 2017.
9.3. Popularization

Nic Volanschi participated on October 12th to the “Science fest” at Inria Bordeaux, where he gave 3 workshop sessions on “Manual digital sciences” for children aged 11 to 15. These workshop sessions were aimed to communicate basic notions of computer science to young students by using puzzles and games.

Antoine Riché and Nic Volanschi presented, to a professional audience coming from various digital-related industries, some of the technologies developed in the team, at the Inria-Industry Meeting on October 17th-18th in Paris centered on “Data and their applications”.

Cécile Mazon participated to the following popularization events:

- “1er Salon du livre et du numérique pour les dys”, on 3rd May 2017. Representing the research center jointly with P.-A. Cinquin (Potioc team); presenting and demonstrating the Collège+ app for iPad.
- “PubHD Bordeaux”, on 24th October 2017. Event consisting in presenting her PhD work “Technologies pour la scolarisation des collégiens avec TSA” without slides nor scientific jargon.
- Guest of the radio show “Que cherchent-ils”, on RCF Bordeaux. 25 minutes for presenting her PhD work around autism and technologies. The show was recorded in December 2017 and will be broadcast in February – March 2018.

10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


International Conferences with Proceedings


Scientific Books (or Scientific Book chapters)


Other Publications


References in notes


Team PLEIADE

from patterns to models in computational biodiversity and biotechnology

Inria teams are typically groups of researchers working on the definition of a common project, and objectives, with the goal to arrive at the creation of a project-team. Such project-teams may include other partners (universities or research institutions).

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Computational Biology
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Diversity, evolution, and inheritance form the heart of modern biological thought. Modeling the complexity of biological systems has been a challenge of theoretical biology for over a century [28] and flourished with the evolution of data for describing biological diversity, most recently with the transformative development of high-throughput sequencing. However, most concepts and tools in ecology and population genetics for capitalizing on this wealth of data are still not adapted to high throughput data production. A better connection between high-throughput data production and tool evolution is highly needed: computational biodiversity.
Paradoxically, diversity emphasizes differences between biological objects, while modeling aims at unifying them under a common framework. This means that there is a limit beyond which some components of diversity cannot be mastered by modeling. We need efficient methods for recognizing patterns in diversity, and linking them to patterns in function. It is important to realize that diversity in function is not the same as coupling observed diversity with function. Diversity informs both the study of traits, and the study of biological functions (Figure 1). The double challenge is to measure these links quickly and precisely with pattern recognition, and to explore the relations between diversity in traits and diversity in function through modeling.

Figure 1. Diversity informs both the study of traits, and the study of biological functions

PLEIADE links recognition of patterns, classes, and interactions with applications in biodiversity studies and biotechnology. We develop distance methods for NGS datasets at different levels of organization: between genomes, between individual organisms, and between communities; and develop high-performance pattern recognition and statistical learning techniques for analyzing the resulting point clouds. We refine inferential methods for building hierarchical models of networks of cellular functions, exploiting the mathematical relations that are revealed by large-scale comparison of related genomes and their models. We combine these methods into integrated e-Science solutions to place these tools directly in the hands of biologists.

Our methodology (Figure 2) is designed pragmatically to advance the state of the art in applications from biodiversity and biotechnology: molecular based systematics and community ecology, annotation and modeling for biotechnology.

Figure 2. PLEIADE is a pluridisciplinary team. Each application in biodiversity and biotechnology follows a path calling on methods from biology (blue), mathematics (green), and computer science (red).

3. Research Program
3.1. A Geometric View of Diversity
Diversity may be studied as a set of dissimilarities between objects. The underlying mathematical construction is the notion of distance. Knowing a set of objects, it is possible, after computation of pairwise distances, or sometimes dissimilarities, to build a Euclidean image of it as a point cloud in a space of relevant dimension. Then, diversity can be associated with the shape of the point cloud. The human eye is often far better than an algorithm at recognizing a pattern or shape. One objective of our project is to narrow the gap between the story that a human eye can tell, and that an algorithm can tell. Several directions will be explored. First, this requires mastering classical tools in dimension reduction, mainly algebraic tools (PCA, NGS, Isomap, eigenmaps, etc ...). Second, neighborhoods in point clouds naturally lead to graphs describing the neighborhood networks. There is a natural link between modular structures in distance arrays and communities on graphs. Third, points (representing, say, DNA sequences) are samples of diversity. Dimension reduction may show that they live on a given manifold. This leads to geometry (differential or Riemannian geometry). It is expected that some properties of the manifold can tell something of the constraints on the space where measured individuals live. The connection between Riemannian geometry and graphs, where weighted graphs are seen as mesh embedded in a manifold, is currently an active field of research [27], [26]. See as well [29] for a link between geometric structure, linear and nonlinear dimensionality reduction.

Biodiversity and high-performance computing: Most methods and tools for characterizing diversity have been designed for datasets that can be analyzed on a laptop, but NGS datasets produced for metabarcoding are far too large. Data analysis algorithms and tools must be revisited and scaled up. We will mobilize both distributed algorithms like the Arnoldi method and new algorithms, like random projection or column selection methods, to build point clouds in Euclidean spaces from massive data sets, and thus to overcome the cubic complexity of computation of eigenvectors and eigenvalues of very large dense matrices. We will also link distance geometry [23] with convex optimization procedures through matrix completion [19], [20].

Intercalibration: There is a considerable difference between supervised and unsupervised clustering: in supervised clustering, the result for an item $i$ is independent from the result for an item $j \neq i$, whereas in unsupervised clustering, the result for an item $i$ (e.g. the cluster it belongs to, and its composition) depends on nearby items $j \neq i$. Which means that the result may change if some items are added to or subtracted from the sample. This raises the more global problem of how to merge two studies to yield a more comprehensive view of biodiversity?

3.2. Knowledge Management for Biology

The heterogenous data generated in computational molecular biology and ecology are distinguished not only by their volume, but by the richness of the many levels of interpretation that biologists create. The same nucleic acid sequence can be seen as a molecule with a structure, a sequence of base pairs, a collection of genes, an allele, or a molecular fingerprint. To extract the maximum benefit from this treasure trove we must organize the knowledge in ways that facilitate extraction, analysis, and inference. Our focus has been on the efficient representation of relations between biological objects and operations on those representations, in particular heuristic analyses and logical inference.

PLEIADE will develop applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on distance geometry will refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities. Since a goal of PLEIADE is to integrate diversity throughout the analysis process, it is necessary to incorporate diversity as a form of knowledge that can be stored in a knowledge base. Diversity can be represented using various compact representations, such as trees and quotient graphs storing nested sets of relations. Extracting structured representations and logical relations from integrated knowledge bases (Figure 2) will require domain-specific query methods that can express forms of diversity.

3.3. Modeling by successive refinement
Describing the links between diversity in traits and diversity in function will require comprehensive models, assembled from and refining existing models. A recurring difficulty in building comprehensive models of biological systems is that accurate models for subsystems are built using different formalisms and simulation techniques, and hand-tuned models tend to be so focused in scope that it is difficult to repurpose them [17]. Our belief is that a sustainable effort in building efficient behavioral models must proceed incrementally, rather than by modeling individual processes de novo. Hierarchical modeling [14] is one way of combining specific models into networks. Effective use of hierarchical models requires both formal definition of the semantics of such composition, and efficient simulation tools for exploring the large space of complex behaviors. We have previously shown that this approach can be effective for certain kinds of systems in biotechnology [2], [18] and medicine [16]. Our challenge is to adapt incremental, hierarchical refinement to modeling organisms and communities in metagenomic and comparative genomic applications.

4. Application Domains

4.1. Genome and transcriptome annotation, to model function

Sequencing genomes and transcriptomes provides a picture of how a biological system can function, or does function under a given physiological condition. Simultaneous sequencing of a group of related organisms is now a routine procedure in biological laboratories for studying a behavior of interest, and provides a marvelous opportunity for building a comprehensive knowledge base of the relations between genomes. Key elements in mining these relations are: classifying the genes in related organisms and the reactions in their metabolic networks, recognizing the patterns that describe shared features, and highlighting specific differences.

PLEIADE will develop applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on computational geometry refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities.

Our ambition in biotechnology is to permit the design of synthetic or genetically selected organisms at an abstract level, and guide the modification or assembly of a new genome. Our effort is focused on two main applications: genetic engineering and synthetic biology of oil-producing organisms (biofuels in CAER, palm oils), and improving and selecting starter microorganisms used in winemaking (collaboration with the ISVV and the BioLaffort company).

4.2. Molecular based systematics and taxonomy

Defining and recognizing myriads of species in biosphere has taken phenomenal energy over the past centuries and remains a major goal of Natural History. It is an iconic paradigm in pattern recognition (clustering has coevolved with numerical taxonomy many decades ago). Developments in evolution and molecular biology, as well as in data analysis, have over the past decades enabled a profound revolution, where species can be delimited and recognized by data analysis of sequences. We aim at proposing new tools, in the framework of E-science, which make possible (i) better exploration of the diversity in a given clade, and (ii) assignment of a place in these patterns for new, unknown organisms, using information provided by sets of sequences. This will require investment in data analysis, machine learning, and pattern recognition to deal with the volumes of data and their complexity.

One example of this project is about the diversity of trees in Amazonian forest, in collaboration with botanists in French Guiana. Protists (unicellular Eukaryots) are by far more diverse than plants, and far less known. Molecular exploration of Eukaryotes diversity is nowadays a standard in biodiversity studies. Data are available, through metagenomics, as an avalanche and make molecular diversity enter the domain of Big Data. Hence, an effort will be invested, in collaboration with other Inria teams (GenScale, HiePACS) for porting to HPC algorithms of pattern recognition and machine learning, or distance geometry, for these tools to be
available as well in metagenomics. This will be developed first on diatoms (unicellular algae) in collaboration with INRA team at Thonon and University of Uppsala), on pathogens of tomato and grapevine, within an existing network, and on bacterial communities, in collaboration with University of Pau. For the latter, the studies will extend to correlations between molecular diversity and sets of traits and functions in the ecosystem.

4.3. Community ecology and population genetics

Community assembly models how species can assemble or disassemble to build stable or metastable communities. It has grown out of inventories of countable organisms. Using metagenomics one can produce molecular based inventories at rates never reached before. Most communities can be understood as pathways of carbon exchange, mostly in the form of sugar, between species. Even a plant cannot exist without carbon exchange with its rhizosphere. Two main routes for carbon exchange have been recognized: predation and parasitism. In predation, interactions—even if sometimes dramatic—may be loose and infrequent, whereas parasitism requires what Claude Combes has called intimate and sustainable interactions [21]. About one decade ago, some works [25] have proposed a comprehensive framework to link the studies of biodiversity with community assembly. This is still incipient research, connecting community ecology and biogeography.

We aim at developing graph-based models of co-occurrence between species from NGS inventories in metagenomics, i.e. recognition of patterns in community assembly, and as a further layer to study links, if any, between diversity at different scales and community assemblies, starting from current, but oversimplified theories, where species assemble from a regional pool either randomly, as in neutral models, or by environmental filtering, as in niche modeling. We propose to study community assembly as a multiscale process between nested pools, both in tree communities in Amazonia, and diatom communities in freshwaters. This will be a step towards community genomics, which adds an ecological flavour to metagenomics.

Convergence between the processes that shape genetic diversity and community diversity—drift, selection, mutation/speciation and migration—has been noted for decades and is now a paradigm, establishing a continuous scale between levels of diversity patterns, beyond classical approaches based on iconic levels like species and populations. We will aim at deciphering diversity pattern along these gradients, connecting population and community genetics. Therefore, some key points must be addressed on reliability of tools.

Next-generation sequencing technologies are now an essential tool in population and community genomics, either for making evolutionary inferences or for developing SNPs for population genotyping analyses. Two problems are highlighted in the literature related to the use of those technologies for population genomics: variable sequence coverage and higher sequencing error in comparison to the Sanger sequencing technology. Methods are developed to develop unbiased estimates of key parameters, especially integrating sequencing errors [24]. An additional problem can be created when sequences are mapped on a reference sequence, either the sequenced species or an heterologous one, since paralogous genes are then considered to be the same physical position, creating a false signal of diversity [22]. Several approaches were proposed to correct for paralogy, either by working directly on the sequences issued from mapped reads [22] or by filtering detected SNPs. Finally, an increasingly popular method (RADseq) is used to develop SNP markers, but it was shown that using RADseq data to estimate diversity directly biases estimates [15]. Workflows to implement statistical methods that correct for diversity biases estimates now need an implementation for biologists.

5. New Software and Platforms

5.1. Magus

**KEYWORDS:** Bioinformatics - Genomic sequence - Knowledge database
**SCIENTIFIC DESCRIPTION:** MAGUS can be used on small installations with a web server and a relational database on a single machine, or scaled out in clusters or elastic clouds using Apache Cassandra for NoSQL data storage and Apache Hadoop for Map-Reduce.
**FUNCTIONAL DESCRIPTION:** The MAGUS genome annotation system integrates genome sequences and sequences features, in silico analyses, and views of external data resources into a familiar user interface requiring only a Web navigator. MAGUS implements annotation workflows and enforces curation standards to guarantee consistency and integrity. As a novel feature the system provides a workflow for simultaneous annotation of related genomes through the use of protein families identified by in silico analyses this has resulted in a three-fold increase in curation speed, compared to one-at-a-time curation of individual genes. This allows us to maintain standards of high-quality manual annotation while efficiently using the time of volunteer curators.

**NEWS OF THE YEAR:** Magus is now available as a Docker image, and can be integrated with other containerized services using Pleiade’s Alcyone system.

- **Participants:** David Sherman, Florian Lajus, Natalia Golenetskaya, Pascal Durrens and Xavier Calcas
- **Partners:** Université de Bordeaux - CNRS - INRA
- **Contact:** David James Sherman
- **Publication:** High-performance comparative annotation
- **URL:** http://magus.gforge.inria.fr

### 5.2. Pantograph

**KEYWORDS:** Systems Biology - Bioinformatics - Genomics - Gene regulatory networks

**SCIENTIFIC DESCRIPTION:** Pantograph requires a template model in SMBL format, where every reaction is annotated with a gene association that describes its gene-protein-reaction dependencies as a boolean formula over the genes of the organism.

Pantograph uses a consensus procedure to infer relationships between metabolic models, based on several sources of orthology between genomes. These inter-genome relations are used to rewrite the gene associations. Every successful rewrite is used as evidence that the corresponding reaction should be present in the inferred model.

The resulting models can be validated with respect to phenotypic information obtained from experimental results.

**FUNCTIONAL DESCRIPTION:** Pantograph is a software toolbox to reconstruct, curate and validate genome-scale metabolic models. It uses existing metabolic models as templates, to start a reconstructions process in which new, species-specific reactions are added. Pantograph uses an iterative approach to improve reconstructed models, facilitating manual curation and comparisons between reconstructed model’s predictions and experimental evidence.

Pantograph uses a consensus procedure to infer relationships between metabolic models, based on several sources of orthology between genomes. This allows for a very detailed rewriting of reaction’s genome associations between template models and the model you want to reconstruct.

**NEWS OF THE YEAR:** Work is in progress to integrate Razanne Issa’s Ab-Pantograph modules into Pantograph. Ab-Pantograph uses abductive logic to invert the inference process: a reaction explains the presence of the genes in its gene-protein-reaction formula, rather than the genes justify the reaction. Ab-Pantograph is driven by the goal of explaining all of the genes in the target organism.

- **Participants:** Anna Zhukova, David James Sherman, Nicolas Loira and Pascal Durrens
- **Partner:** University of Chile
- **Contact:** Nicolas Loira
- **Publication:** Pantograph: A template-based method for genome-scale metabolic model reconstruction
- **URL:** http://pathtastic.gforge.inria.fr/
5.3. Mimoza

**KEYWORDS:** Systems Biology - Bioinformatics - Biotechnology

**FUNCTIONAL DESCRIPTION:** Mimoza uses metabolic model generalization and cartographic paradigms to allow human experts to explore a metabolic model in a hierarchical manner. Mimoza generalizes genome-scale metabolic models, by factoring equivalent reactions and metabolites while preserving reaction consistency. The software creates an zoomable representation of a model submitted by the user in SBML format. The most general view represents the compartments of the model, the next view shows the visualization of generalized versions of reactions and metabolites in each compartment, and the most detailed view visualizes the initial model with the generalization-based layout (where similar metabolites and reactions are placed next to each other). The resulting map can be explored on-line, or downloaded in a COMBINE archive. The zoomable representation is implemented using the Leaflet JavaScript library for mobile-friendly interactive maps. Users can click on reactions and compounds to see the information about their annotations.

**NEWS OF THE YEAR:** Mimoza is now available as a Docker image, and can be integrated with other containerized services using Pleiade’s Alcyone system.

- Participants: Anna Zhukova and David James Sherman
- Contact: David James Sherman
- Publications: Knowledge-based generalization of metabolic models - Knowledge-based zooming for metabolic models - Knowledge-based generalization of metabolic networks: a practical study
- URL: http://mimoza.bordeaux.inria.fr/

5.4. Declic

**FUNCTIONAL DESCRIPTION:** Declic is a Python library that provides several tools for data analysis in the domains of multivariate data analysis, machine learning, and graph based methods. It can be used to study in-depth the accuracy of the dictionary between molecular based and morphological based taxonomy. Declic includes an interpreter for a Domain Specific Language (DSL) to make its Python library easy to use for scientists familiar with environments such as R.

- Partner: INRA
- Contact: Alain Franc

5.5. Diagno-Syst

*diagno-syst: a tool for accurate inventories in metabarcoding*

**KEYWORDS:** Biodiversity - Clustering - Ecology

**FUNCTIONAL DESCRIPTION:** Diagno-syst builds accurate inventories for biodiversity. It performs supervised clustering of reads obtained from a next-generation sequencing experiment, mapping onto an existing reference database, and assignment of taxonomic annotations.

- Participants: Alain Franc, Jean-Marc Frigerio, Philippe Chaumeil and Franck Salin
- Partner: INRA
- Contact: Alain Franc
- Publication: diagno-syst: a tool for accurate inventories in metabarcoding

5.6. Alcyone

*Alcyone instantiates bioinformatics environments from specifications committed to a Git repository*

**KEYWORDS:** Docker - Orchestration - Bioinformatics - Microservices - Versioning
SCIENTIFIC DESCRIPTION: Alcyone conceives the user’s computing environment as a microservices architecture, where each bioinformatics tool in the specification is a separate containerized Docker service. Alcyone builds a master container for the specified environment that is responsible for building, updating, deploying and stopping these containers, as well as recording and sharing the environment in a Git repository. The master container can be manipulated using a command-line interface.

FUNCTIONAL DESCRIPTION: Alcyone defines a file structure for the specifying bioinformatics analysis environments, including tool choice, interoperability, and sources of raw data. These specifications are recorded in a Git repository. Alcyone compiles a specification into a master Docker container that deploys and orchestrates containers for each of the component tools. Alcyone can restore any version of an environment recorded in the Git repository.

NEWS OF THE YEAR: Alcyone was designed and implemented this year.
- Participants: Louise-Amelie Schmitt and David Sherman
- Contact: David Sherman
- URL: https://team.inria.fr/pleiade/alcyone/

6. New Results

6.1. Alcyone system for repeatable e-science

One of PLEIADE’s goals is to assist scientific users in deploying analysis software in their desktop environments. Increasingly, this is not a question of installing software packages locally, but of building bespoke environments that comprise many cooperating software tools. A typical example is a local Galaxy instance, communicating with a project-specific database that is shared with visualization and analysis tools, and cooperating with an electronic notebook such as Jupyter. In order to foster repeatable science, the configuration of each such environment should be reliably recorded, in a way that allows it to be redeployed in the future or shared with a colleague.

PLEIADE’s Alcyone system provides a mechanism for specifying and deploying software environments for scientific users in bioinformatics and biodiversity. Alcyone offers three facilities:

2. A collection of Dockerized services that can be chosen in the specification.
3. A deployment system that compiles the specification into a master container image, which orchestrates the deployment and management of the service containers.

The user’s environment is fully specified in files that can be archived and shared, allowing future reuse. The use of Docker containers guarantees that future deployments run exactly as before, since the precise versions of the service containers are recorded.

Furthermore, Alcyone specifications are files, that can be managed by the Git source code control system. Different versions of the environment, including different analysis pipelines and intermediate results, are stored in the Git history and any version can be resurrected and deployed. Git branches can also be used to share configurations between users in the same lab.

Alcyone is being tested internally by PLEIADE and is undergoing intense development. Existing service containers are PLEIADE’s Magus knowledge base, Magecal gene prediction pipeline, and Mimoza metabolic network explorer; as well as third-party tools Galaxy, Gbrowse, and Jbrowse.
6.2. Clavispora lusitaniae

*Clavispora lusitaniae*, an environmental saprophytic yeast belonging to the CTG clade of *Candida* and a teleomorph of *Candida lusitaniae*, is an environmentally ubiquitous ascomycetous yeast with no known specific ecological niche. It can be isolated from different substrates, such as soils, waters, plants, and gastrointestinal tracts of many animals including birds, mammals, and humans. In immunocompromised hosts, *C. lusitaniae* can be pathogenic and is responsible for about 1% of invasive candidiasis, particularly in pediatric and hematology-oncology patients.

The Laboratoire de Microbiologie Fondamentale et Pathogénicité UMR-CNRS 5234 and PLEIADE sequenced and annotated the genome of *C. lusitaniae* type strain CBS 6936, and analyzed it in comparison with the strains ATCC 42720, isolated from the blood of a patient with myeloid leukemia, and MTCC 1001, a self-fertile strain isolated from citrus. In spite of a conserved genome structure, the genomes have undergone significant divergence. In particular the SNP density of 1 SNP per 90 bp is twice the level observed between strains SC5314 and WO-1 of *Candida albicans*, which are members of different subgroups within the species and qualified as having diverged relatively recently.

This work contributes to PLEIADE’s long-term goal of developing understanding how diversity measured at the genome level can be made to correspond with observed functional diversity.

6.3. Introgressions as a source of diversity

Several prominent mechanisms of genomic evolution have been described for the yeasts, among them inter-specific hybridization, reticulated evolution, aneuploidization, recent or ancient poly-ploidization events, large chromosomal duplication or more limited gene duplication, and horizontal transfer. These mechanisms are usually so closely intertwined that it is difficult to determine which ones are causes or consequences. Regardless of mechanisms the result has been a drastic reshaping of yeasts genome along evolution. Understanding these mechanisms is important, not only for strain construction in biotechnology, but also more fundamentally for insight into the causes and effects of genome reshaping on much shorter time scales.

Introgression, the transfer of large or more limited genetic information from one species to another, is an evolutionary mechanism of particular interest in industrial applications such as wine making where large vat cultures are used. Introgression results in mosaic genomes, and can be the result of interspecific hybridization followed by the extensive loss of one parental genome, either through repeated backcross with one parental species or through missegregation of the hybrid at meiosis.

In collaboration with the Institut des Science de la Vigne et du Vin and Bordeaux Sciences Agro, PLEIADE developed tools to rapidly assess the presence of introgressed regions in a large population of *Saccharomyces uvarum* isolates (104 strains), focusing on Holarctic isolates from natural, cider and wine environments since introgressed regions are absent in Southern hemisphere isolates. The overall number of introgressed regions is significantly higher in cider-associated strains compared to wild strains, and is higher in wine isolates. However, only a subset of the introgressed regions were found to be overrepresented in anthropic activities and their number and quality varied between cider- and wine-making processes.

Paradoxically, the low Holarctic genetic diversity observed in [1] contrasts with the relative high phenotypic diversity found for technological traits. This contradiction suggests that interspecific introgressions found among Holarctic *S. uvarum* strains could be the most important source of genetic, and by extention of phenotypic, diversity.

6.4. New results Biodiversity

The activity of PLEIADE in computational biodiversity has consisted mainly in reinforcing a cooperation with actors in High Performance Computing, namely Inria team Hiepacs, for method developments in metabarcoding. Metabarcoding is a supervised or unsupervised statistical learning method, to build taxonomic inventories from so called environmental samples, i.e. sets of short reads of a same marker for a whole community or guild. Most of tools used therefore still rely on some classical ones shaped in Multivariate
Data Analysis. Those tools are indeed well known, but still are often behind the scene in current developments in Machine Learning (like kernel PCA, Support Vector Machines, etc.). Most of them, if not all, are based on Singular Value Decomposition of a matrix. If \( p \) features are observed on \( n \) items, the size of the matrix is \( n \times p \). The complexity of such algorithms is in \( O(p^3) \). The recent development of NGS data has had as a consequence to multiply by a factor \( 10^2/10^3 \) the size of data sets. This leads to a factor \( 10^6/10^9 \) of required computation time. Reaching such a goal is beyond resources currently offered by parallelization. Hence, a new approach has been selected, by using other methods. Indeed, it has been known for some years now that concentration of measure phenomena (a sort of extension of law of large numbers) leads to a blessing of dimensionality, i.e. some randomized methods are available as heuristics to make some matrix computations efficiently and accurately. This is the case for running SVD. Therefore, a cooperation has been set up between HiePacs and PLEIADE through Pierre Blanchard (a former Hiepacs PhD student who has held a post-doc position during 7 months in PLEIADE) to implement those methods in the framework of metabarcoding. Former work in PLEIADE had led (with a DARI project 2014-2016) to the production of many high-dimensional pairwise distance matrices of DNA environmental samples (amplicon based metabarcoding). Classical Multidimensional Scaling of some of those matrices has been programmed in C++, with dedicated libraries in domain of so called random projection, or column selection (fmr library). This has permitted to build a point cloud of an environmental sample of \( 1.2 \times 10^5 \) reads, and see its “shape”, with eyes, from projections on first axis, and build a low dimensional approximation of it. The outcome is twofolds: (i) build a point cloud attached to an environmental sample, for further ecological studies and (ii) delivery of a scientific library in High Performance Computing for randomized matrix computations. These research lines will be carried on in 2018, and the cooperation extended to mésocentre GRICAD in Grenoble for HPC and C++ code development.

PLEIADE has carried on statistical learning methods, both supervised and unsupervised in metabarcoding. A cooperation with IMBE at Marseille has permitted to associate MDS as developed above with graph based methods (building connected components of a graph built from pairwise distance matrices after thresholding), and test these methods for unsupervised statistical learning (OTU building) of data sets from an ongoing PhD in Marseille Bay. Cooperation with Institut Pasteur at Cayenne has lead to a joint publication [12] for a proof of concept of an inventory by metagenomics of viromes of bats in French Guiana, with two objectives: (i) detect as soon as possible some strains which could potentially be transmitted to man and (ii) develop a viral ecology by studying further how environmental factors and nature of the host drive the virome composition.

Meanwhile, PLEIADE has carried on cooperation with SLU Universty at Uppsala especially on metabarcoding of diatom communities in rivers and lakes in Sweden (co-direction of a PhD student located at Uppsala in SLU), and first steps in biogeography of diatoms in Fennoscandia (cooperation with a PostDoc in SLU).

7. Partnerships and Cooperations

7.1. Regional Initiatives

7.1.1. COTE – Continental to Coastal Ecosystems

The Labex cluster of excellence COTE (Continental To coastal Ecosystems: evolution, adaptability and governance) develops tools to understand and predict ecosystem responses to human-induced changes as well as methods of adaptive management and governance to ensure their sustainability. The LabEx includes nine laboratories of the University of Bordeaux and major national research institutes involved in research on terrestrial and aquatic ecosystems (INRA, CNRS, IFREMER and IRSTEA). PLEIADE is a partner in one project funded by COTE:

7.2. National Initiatives

7.2.1. Biocontamination in aircraft reservoirs

ANTICOR is an industrial-academic research and development working group coordinated by Dassault Aviation, investigating the causes of microbial contamination in aircraft reservoirs and aimed at developing mitigating procedures and equipment. Previous results have shown that this contamination forms biofilms at the fuel-water interface and is comprised of complex communities of hundreds of bacterial and fungal species. PLEIADE is particularly interested in measuring and modeling these communities, especially as concerns understanding how they change based on environmental conditions and on reservoir geometry.

This working group continues work started in CAER – Alternative Fuels for Aeronautics, a 6 M-Euro contract with the Civil Aviation Directorate (Direction Générale de l’Aviation Civile, DGAC), coordinated by the French Petroleum Institute (Institut français de pétrole-énergies nouvelles, IFPEN) on behalf of a large consortium of industrial (EADS, Dassault, Snecma, Turbomeca, Airbus, Air France, Total) and academic (CNRS, INRA, Inria) partners to explore different technologies for alternative fuels for aviation.

7.2.2. Agence Française pour la Biodiversité

The AFB is a public law agency of the French Ministry of Ecology that supports public policy in the domains of knowledge, preservation, management, and restoration of biodiversity in terrestrial, aquatic, and marine environments. PLEIADE is a partner in two AFB projects developed with the former ONEMA:

- **Methods for metabarcoding.** 2017-18.
- **Molecular diagnosis of freshwater quality.** 2014-present.

7.2.3. Inria Projet Lab in silico Algae

In 2017 PLEIADE joined the IPL “In silico Algae” coordinated by Olivier Bernard. The IPL addresses challenges in modeling and optimizing microalgae growth for industrial applications. PLEIADE worked this year on comparative genomic analysis of genes implicated in lipid production by the picocalgae *Ostreococcus tauri*, in collaboration with Florence Corellou of the CNRS UMR 5200 (Laboratoire de Biogénèse Membranaire). The goal of this work is the production of long-chain polyunsaturated fatty acids, developed as nutritional additives. Mercia Ngoma Komb’s two-month internship in PLEIADE contributed to this work.

7.3. European Initiatives

7.3.1. Collaborations in European Programs, Except FP7 & H2020

Alain Franc has been appointed co-chair of Working Group 4 (Data Analysis and Storage) of COST DNAqua.net at the Sarajevo meeting in Fall 2017, with the main task of developing contact with HPC and metabarcoding for serving the whole community. The goal of DNAqua-Net is to nucleate a group of researchers across disciplines with the task to identify gold-standard genomic tools and novel eco-genomic indices and metrics for routine application for biodiversity assessments and biomonitoring of European water bodies.

7.4. International Initiatives

7.4.1. CEBA – Center for the study of biodiversity in Amazonia

The Laboratoire of excellence CEBA promotes innovation in research on tropical biodiversity. It brings together a network of internationally-recognized French research teams, contributes to university education, and encourages scientific collaboration with South American countries. PLEIADE participates in three current international projects funded by CEBA:

- **MicroBIOMES: Microbial Biodiversities.** 2017-19.
- **Neutrophyl: Inferring the drivers of Neotropical diversification.** 2017-19.
- **Phyloguianas: Biogeography and pace of diversification in the Guiana Shield.** 2015-present

0http://dnaqua.net/
8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific Events Organisation

8.1.1.1. General Chair, Scientific Chair

Alain Franc organized on September 25-29, 2017 an ANF (Action Nationale de Formation) of CNRS on “Data analysis for massive data”. There were about 20 participants, from Astronomy to Bioinformatics, over Fluid Mechanics.

8.1.2. Journal

8.1.2.1. Member of Editorial Boards

Alain Franc is member of the editorial board of BMC Evolutionary Biology.

Pascal Durrens is a member of the editorial board of the journal ISRN Computational Biology.

8.2. Teaching - Supervision - Juries

8.2.1. Juries

David Sherman was a thesis reviewer for Julie Laniau (University of Nantes) and member of her defense jury, October 23, 2017. The title of the dissertation was “Structure de réseaux biologiques : rôle des nœuds internes vis-a-vis de la production de compose’s” and concerned the methodological analysis of metabolite essentiality in metabolic modeling, applied to algae.

Alain Franc was a thesis reviewer for Cyril Noël (University of Pau and the Pays d’Adour) and member of his defense jury, 2017. The title of the dissertation was “Réseaux microbiens de dégradation des hydrocarbures aux interfaces oxie/anoxie des sédiments marins côtiers” and concerned metabarcoding, metagenomics and functional metagenomics of some Bactera and Archea.

Alain Franc was president of the jury for PhD defense of Pierre Blanchard (University of Bordeaux and Inria project-team HiePACS) on February 16, 2017. The title of the dissertation was “Fast hierarchical algorithms for the low-rank approximation of matrices with applications to materials physics, geostatistics and data analysis”

8.3. Popularization

David Sherman of PLEIADE coached two teams in Thymio R2T2 Challenges 0, organized by the Mobsya association and the EPFL in Spring and in Summer 2017. An R2T2 challenge brings together 16 teams (for the Mars mission, 4 teams for the Lunar mission) of children who must cooperate to remotely program Thymio robots. The Lunar mission in July was a public demonstration during the Scratch 2017 conference in Bordeaux.

David Sherman contributes open-source software development to the Aseba platform for educational robotics 0, deployed in Thymio II robots used by children as well as in the simulator used by Class’Code 0 to train teachers.

---

0Remote Rescue Thymio II https://www.thymio.org/en/thymio-r2t2
0http://aseba.io/
0https://pixees.fr/classcode-la-formation-associee-a-pixees/
9. Bibliography

Major publications by the team in recent years


Publications of the year

Articles in International Peer-Reviewed Journal


Research Reports


References in notes


Project-Team POTIOC

Popular interaction with 3d content

IN PARTNERSHIP WITH:
CNRS
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Interaction and visualization
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Project-Team POTIOC

Creation of the Team: 2012 January 01, updated into Project-Team: 2014 January 01

Keywords:

**Computer Science and Digital Science:**
- A3.2.2. - Knowledge extraction, cleaning
- A3.4.1. - Supervised learning
- A5.1. - Human-Computer Interaction
- A5.1.1. - Engineering of interactive systems
- A5.1.2. - Evaluation of interactive systems
- A5.1.4. - Brain-computer interfaces, physiological computing
- A5.1.5. - Body-based interfaces
- A5.1.6. - Tangible interfaces
- A5.1.7. - Multimodal interfaces
- A5.1.8. - 3D User Interfaces
- A5.6. - Virtual reality, augmented reality
- A5.9. - Signal processing
- A5.9.2. - Estimation, modeling
- A9.2. - Machine learning
- A9.3. - Signal analysis

**Other Research Topics and Application Domains:**
- B1.2. - Neuroscience and cognitive science
- B2.1. - Well being
- B2.5.1. - Sensorimotor disabilities
- B2.5.2. - Cognitive disabilities
- B2.6.1. - Brain imaging
- B5.2.4. - Aerospace
- B9.1. - Education
- B9.1.1. - E-learning, MOOC
- B9.2. - Art
- B9.2.1. - Music, sound
- B9.4.3. - Physics
- B9.5.1. - Psychology
- B9.5.7. - Geography

1. Personnel

**Research Scientists**
- Martin Hachet [Team leader, Inria, Researcher, HDR]
- Anke Brock [Inria, Researcher, until Sep 2017]
- Fabien Lotte [Inria, Researcher, HDR]

**Faculty Member**
2. Overall Objectives

2.1. Overall Objectives

The overall objective of Potioc is to design, to develop, and to evaluate new approaches that provide rich interaction experiences between users and the digital world. Thus, we aim at stimulating motivation, curiosity, engagement, or pleasure of use. In other words, we are interested in popular interaction, mainly targeted at the general public.

We believe that such popular interaction may enhance learning, creation, entertainment or popularization of science that are the main application areas targeted by our project-team. To this end, we explore input and output modalities that go beyond standard interaction approaches which are based on mice/keyboards and (touch)screens. Similarly, we are interested in 3D content that offers new opportunities compared to traditional 2D contexts. More precisely, Potioc explores interaction approaches that rely notably on interactive 3D graphics, augmented and virtual reality (AR/VR), tangible interaction, brain-computer interfaces (BCI) and physiological computing.

Such approaches hold great promises in a number of fields. For example, interactive 3D graphics have become ubiquitous in the industry, where they have revolutionized usages, notably by improving work cycles for conception or simulation tasks. However, except for video games, we believe that such approaches are still far from being exploited to their full extent outside such industrial contexts despite having a huge potential for the masses in the areas targeted by our project.

In order to design interactive systems that can be beneficial to many people, and not only expert users, we propose to change the usual design approaches that are generally driven by criteria such as speed, efficiency or precision. Instead, we give more credit to the user experience, in particular criteria such as interface appeal and enjoyment arising from the interface use. Indeed, these criteria have been often neglected in academic research whereas we believe they are crucial for users who are novices with 3D interaction, multisensory spaces, or brain-computer interfaces. An interface with a strong appeal and enjoyment factor will motivate users to use and benefit from the system.
3. Research Program

3.1. Introduction

The project of team potioc is oriented along three axes:

- Understanding humans interacting with the digital world
- Creating interactive systems
- Exploring new applications and usages

These axes are depicted in Figure 2.

Objective 1 is centered on the human sensori-motor and cognitive abilities, as well as user strategies and preferences, for completing interaction tasks. Our target contribution for this objective are a better understanding of humans interacting with interactive systems. The impact of this objective is mainly at a fundamental level.

In objective 2, our goal is to create interactive systems. This may include hardware parts where new input and output modalities are explored. This also includes software parts, that are strongly linked to the underlying hardware components. Our target contribution in objective 2 is to develop (hardware/software) interaction techniques allowing humans to perform interaction tasks.

Finally, in objective 3, we consider interaction at a higher level, taking into account factors that are linked to specific application domains and usages. Our target contribution in this area is the exploration and the emergence of new applications and usages that take benefit from the results of the project. With this objective, we target mainly a societal impact.
Of course, strong links exist between the three objectives of the project. For example, the results obtained in objective 1 guide the development of objective 2. Conversely, new systems developed in objective 2 may feed research questions of objective 1. There are similar links with objective 3.

3.2. Objective 1: Understanding humans interacting with the digital world

Our first objective is centered on the human side. Our finality is not to enhance the general knowledge about the human being as a research team in psychology would do. Instead, we focus on human skills and behaviors during interaction processes. To this end, we conduct experiments that allow us to better understand what users like, where and why they have difficulties. Thanks to these investigations, we are able to design interaction techniques and systems (described in Objective 2) that are well suited to the targeted users. We believe that this fundamental piece of work is the first step that is required for the design of usable popular interactions. We are particularly interested in 3D interaction tasks for which we design dedicated experiments. We also explore a new approach based on physiological and brain (ElectroEncephaloGraphy - EEG) signals for the evaluation of these interactions.

3.2.1. Interacting with physical and virtual environments

Interacting with digital content displayed on 2D screens has been extensively studied in HCI. On the other hand, less conventional contexts have been studied less. This is the case of 3D environments, immersive virtual environments, augmented reality, and tangible objects. With the final goal of making interaction in such contexts user-friendly, we conduct experiments to better understand user strategies and performance. This allows us to propose guidelines to help designers creating of tools that are accessible to non-expert users.

3.2.2. Evaluating (3D) interaction with physiological signals

Recently, physiological computing has been shown to be a promising complement to Human-Computer Interfaces (HCI) in general, and to 3D User Interfaces (3DUI) in particular, in several directions. Within this research area, we are interested in using various physiological signals, and notably EEG signals, as a new tool to assess objectively the ergonomic quality of a given (3D) UI, to identify where and when are the pros and cons of this interface, based on the user’s mental state during interaction. For instance, estimating the user’s mental workload during interaction can give insights about where and when the interface is cognitively difficult to use. This could be useful for 2D HCI in general, and even more for 3DUI. Indeed, in a 3DUI, the user perception of the 3D scene – part of which could potentially be measured in EEG - is essential. Moreover, the usual need for a mapping between the user inputs and the corresponding actions on 3D objects make 3DUI and interaction techniques more difficult to assess and to design.
3.2.3. Interacting with Brain-Computer Interfaces

Although very promising for numerous applications, BCIs mostly remain prototypes not used outside laboratories, due to their low reliability. Poor BCI performances are partly due to imperfect EEG signal processing algorithms but also to the user who may not be able to produce reliable EEG patterns. Indeed, BCI use is a skill, requiring the user to be properly trained to achieve BCI control. If he/she cannot perform the desired mental commands, no signal processing algorithm can identify them. Therefore, rather than improving EEG signal processing alone, an interesting research direction is to also guide users to learn BCI control mastery. We aim at addressing this objective. We are notably exploring theoretical models and guidelines from educational sciences to improve BCI training protocols. We also study which users’ profiles (personality and cognitive profile) fail or succeed at learning BCI control. Finally, we explore new feedback types and new EEG visualization techniques in order to help users gain BCI control skills more efficiently. These new feedback and visualizations notably aim at providing BCI users with more information about their EEG patterns, in order to identify more easily relevant BCI control strategies, as well as motivating and engaging them in the learning task.

3.2.4. Interaction for people with special needs

Interaction capabilities and needs largely depend on the target user group. In the Potioc project-team, we work with people having special needs. As an example, we work with children in the context of education, which requires us to design interfaces that are usable, engaging and support learning for this target group. Furthermore, we work with people with cognitive or perceptive disabilities, which requires us to consider accessibility, while at the same time designing interfaces that are learnable and enjoyable to use. In order to meet the needs of the different target groups, we apply participative and user-centred design methods.

3.3. Objective 2: Creating interactive systems

Our objective here is to create interactive systems and design interaction techniques dedicated to the completion of interaction tasks. We divide our work into three main categories:

- Interaction techniques based on existing Input/Output (IO) devices.
- New IO and related techniques.
- BCI and physiological computing.

3.3.1. Interaction techniques based on existing Input/Output (IO) devices

When using desktop IOs (i.e., based on mice/keyboards/monitors), a big challenge is to design interaction techniques that allow users to complete 3D interaction tasks. Indeed, the desktop IO space that is mainly dedicated to the completion of 2D interaction task is not well suited to 3D content and, consequently, 3D user interfaces need to be designed with a great care. In the past few years, we have been particularly interested in the problem of interaction when the 3D content is displayed on a touchscreen. Indeed, standard (2D) HCI has evolved from mouse to touch input, and numerous research projects have been conducted. On the contrary, in 3D, very little work has been proposed. We are contributing to moving desktop 3D UIs from the mouse to the touch paradigm; what we used to do with mice in front of a screen does not work well on touch devices anymore. In the future, we will continue designing new interaction techniques that are based on standard IOs (eg. pointing devices and webcams) and that target the main objectives of Potioc which are to enhance the interaction bandwidth for non expert users.

3.3.2. New IO and related techniques

Beyond standard IOs, we are interested in exploring new IO modalities that may make interaction easier, more engaging and motivating. In Potioc, we design new interactive systems that exploit unconventional IO modalities such as stereoscopy, 3D spatial input, augmented reality and so on. In particular, tangible interaction and spatial augmented reality are major subjects of interest for us. Indeed, we believe that manipulating directly physical objects for interacting with the digital world has a great potential, in particular when the general public is targeted. With such approaches, the computer disappears, and the user interacts with the digital content as he
or she would do with physical content, which reduces the distance to the manipulated content. As an example, we recently designed Teegi, a new system based on a unique combination of spatial augmented reality, tangible interaction and real-time neurotechnologies. With Teegi, a user can visualize and analyze his or her own brain activity in real-time, on a tangible character that can be easily manipulated, and with which it is possible to interact. Such unconventional user interfaces that are based on rich sensing modalities hold great promises in the field of popular interaction.

We are also interested in designing systems that combine different sensory modalities, such as vision, touch and audition. Concrete examples include the design of tangible user interfaces or interfaces for visually impaired people. It has been shown that multimodality can provide rich interaction that can efficiently support learning, and it is also important in the context of accessibility.

3.3.3. BCI and physiological computing

Although Brain-Computer Interfaces (BCI) have demonstrated their tremendous potential in numerous applications, they are still mostly prototypes, not used outside laboratories. This is mainly due to the following limitations:

- Performances: the poor classification accuracies of BCIs make them inconvenient to use or simply useless compared to available alternatives
- Stability and robustness: the sensibility of ElectroEncephaloGraphic (EEG) signals to noise and their inherent non-stationarity make the already poor initial performances difficult to maintain over time
- Calibration time: the need to tune current BCIs to each user’s EEG signals makes their calibration times too long.

As part of our research on EEG-based BCIs, we notably aim at addressing these limitations by designing robust EEG signal processing tools with minimal calibration times, in order to design practical BCI systems, usable and useful outside laboratories. To do so we explore the design of alternative features and robust spatial filtering algorithms to make BCIs more robust to noise and non-stationarities, as well as more accurate. We also explore artificial EEG data generation and user-to-user data transfer to reduce calibration times.

3.4. Objective 3: Exploring new applications and usages

Objective 3 is centered on the applications and usages. Beyond the human sensori-motor and cognitive skills (Objective 1), and the hardware and software components (Objective 2), Objectives 3 takes into account broader criteria for the emergence of new usages and applications in various areas, and in particular in the scope of education, art, popularization of science and entertainment. Our goal here is not to develop full-fledged end-user applications. Instead, our contribution is to stimulate the evolution of current applications with new engaging interactive systems.

3.4.1. Education

Education is at the core of the motivations of the Potioc group. Indeed, we are convinced that the approaches we investigate—which target motivation, curiosity, pleasure of use and high level of interactivity—may serve education purposes. To this end, we collaborate with experts in Educational Sciences and teachers for exploring new interactive systems that enhance learning processes. We are currently investigating the fields of astronomy, optics, and neurosciences. We are also working with special education centres for the blind on accessible augmented reality prototypes. In the future, we will continue exploring new interactive approaches dedicated to education, in various fields.

3.4.2. Popularization of science

Popularization of Science is also a key domain for Potioc. Focusing on this subject allows us to get inspiration for the development of new interactive approaches. In particular, we have built a strong partnership with Cap Sciences, which is a center dedicated to the popularization of science in Bordeaux that is visited by thousands of visitors every month. This was initiated with the ANR national project InSTInCT, whose goal was to study the benefits of 3D touch-based interaction in public exhibitions. This project has led to the creation of a Living
Lab where several systems developed by Potioc have been tested and will be tested by the visitors. This provides us with very interesting observations that go beyond the feedback we can obtain in our controlled lab-experiments.

### 3.4.3. Art

Art, which is strongly linked with emotions and user experiences, is also a target area for Potioc. We believe that the work conducted in Potioc may be beneficial for creation from the artist point of view, and it may open new interactive experiences from the audience point of view. As an example, we are working with colleagues who are specialists in digital music, and with musicians. We are also working with jugglers and mockup builders with the goal of enhancing interactivity and user experience.

### 3.4.4. Entertainment

Similarly, entertainment is a domain where our work may have an impact. We notably explored BCI-based gaming and non-medical applications of BCI, as well as mobile Augmented Reality games. Once again, we believe that our approaches that merge the physical and the virtual world may enhance the user experience. Exploring such a domain will raise numerous scientific and technological questions.

### 4. Application Domains

#### 4.1. Education, popularization of science, art, entertainment

Our project aims at providing rich interaction experiences between users and the digital world, in particular for non-expert users. The final goal is to stimulate understanding, learning, communication and creation. Our scope of applications encompasses

- education
- popularization of science
- art
- entertainment

See "Objective 3: Exploring new applications and usages“ (3.4) for a detailed description.

### 5. Highlights of the Year

#### 5.1. Highlights of the Year

- A Handbook of Brain-Computer Interfaces was co-edited by Potioc (F. Lotte), involving the international BCI community [41]

##### 5.1.1. Awards

- Best paper - Honorable mention award (top 5% over 2400 submissions), ACM CHI 2017, HOBIT, D. Furio, S. Fleck, B. Bousquet, J.-P. Guillet, L. Canioni, M. Hachet
- Best paper - Honorable mention award (top 5% over 2400 submissions), ACM CHI 2017, Inner Garden, J. S. Roo, R. Gervais, J. Frey, M. Hachet
- Honorable mention award, MUM’17, Bespoke map customization, A. Brock, B. Hecht, B. Signer, J. Schöning
- Best technote award, IEEE 3DUI 2017, Hybrid space, J. S. Roo, M. Hachet
- Best Demo award for Teegi, IHM 17, T. Lainé, J. Frey, M. Hachet
- PhD thesis award, International PhD award committee from Bordeaux University 2017, C. Jeunet
- PhD thesis award, IFRATH/KAELIS 2017, C. Jeunet
- 2 Publons top peer reviewer awards in 2017, for the top 1% most peer reviews in both Engineering in Neuroscience, F. Lotte

**BEST PAPERS AWARDS**
6. New Software and Platforms

6.1. Aïana

**KEYWORD:** Multimedia player

**FUNCTIONAL DESCRIPTION:** This software aims to make accessible the playing of a MOOC composed of various information flows (boards, videos, subtitles ...). It is not intended to be "reserved" for people with disabilities but rather to open to as many as possible by allowing each user to adapt the interface, and therefore the use, to its own capabilities and needs.

- **Authors:** Marc Chambon, Julien Grynberg, Hélène Sauzéon, Pascal Guittion and Pierre-Antoine Cinquin
- **Partner:** Université de Bordeaux
- **Contact:** Pascal Guittion

6.2. HybridOptics: Hybrid Optical Platform

**KEYWORDS:** Augmented reality - Education - Tangible interface

**FUNCTIONAL DESCRIPTION:** The software platform - gets the values of the sensors - computes in real-time the result of the simulation - generates pedagogical supports that are directly linked to the simulation (projected on the work table) - allows the user to control several parameters from a dedicated application on a tablet

- **Participants:** Benoît Coulais, Lionel Canioni, Bruno Bousquet, Martin Hachet and Jean-Paul Guillet
- **Contact:** Martin Hachet
- **URL:** https://project.inria.fr/hobit/fr/

7. New Results

7.1. HOBIT

**Participants:** David Furio, Benoit Coulais, Martin Hachet

Practical work in optics learning allows supporting the construction of knowledge, in particular when the concept to be learned remains diffuse. To overcome the limitations of the current experimental setups, we have designed a hybrid system that combines physical interaction and numerical simulation. This system relies on 3D-printed replicas of optical elements, which are augmented with pedagogical information (see Figure 3). In a first step, we have focused on the well-known Michelson interferometer experiment, widely studied in graduate programs of Science. A 3-months user study with 101 students and 6 teachers showed that, beyond the practical aspects offered by this system, such an approach enhances the technical and scientific learning compared to a standard Michelson interferometer experiment. This work has been published at CHI 2017 [24], and the paper obtained a Best Paper - Honorable Mention Award.

Currently, we are developing a second version of HOBIT. This new version will let us simulate and augment multiple experiments related with optics, like polarization or Young’s interferometer.
7.2. Inner Garden

Participants: Joan Sol Roo, Renaud Gervais, Jeremy Frey, Martin Hachet

Digital technology has completely integrated our daily lives; we use it for entertainment, productivity and our social lives. However, the potential of leveraging technology to improve its users’ overall happiness and life satisfaction is still largely untapped. Mindfulness, the act of paying a deliberate and non-judgmental attention to the present moment, has been shown to have a positive impact on a person’s subjective well-being. With this in mind we created Inner Garden, an ambient mixed reality installation, inspired by a zen garden, comprised of an augmented sandbox along with a virtual reality modality to support mindful experiences (Figure 4). By shaping the sand, the user creates a living miniature world that is projected back onto the sand. Moreover, using a VR headset, she can take a moment to herself by actually going inside her own garden to meditate. The natural elements of the garden are connected to real-time physiological measurements, such as breathing, helping staying focused on the body. We evaluated the system through a first user study and consulted meditation teachers, who envisioned the use of the garden in their teaching, especially for novice practitioners. The reception of the system seems to indicate that technology can, when designed carefully, both engage the users and foster well-being.

This work has been published at CHI 2017 [32], and the paper obtained a Best Paper - Honorable Mention Award.
7.3. Art and Science

Participants: Clémentine Petit, Maxime Agor, Martin Hachet

Potioc collaborates with artists for Art and Science projects. These projects are supported by a dedicated program at Idex - Université de Bordeaux.

The first one, Kilometre 2.0, is a joint project with Cécile Léna https://www.lenadazy.fr who is a visual artist and scenographer. We have augmented physical mockups with digital objects (see Figure 5). More concretely, our system detects train tickets being manipulated above a miniature scenery. Depending on their locations, dedicated movies are projected exactly on them, in the 3D space. Other sound and smoke effects are also generated. This artistic and interactive setup has been showed during the FACTS festival in November 18.

![Figure 5. Spatial augmented reality in an artistic installation](image)

The second project is conducted in collaboration with Antoine Clée from Le Cirque Inachevé http://www.lecirqueinacheve.fr. Our objective is to explore new forms of juggling where the balls are not constrained by gravity anymore. More precisely, the balls are held by nano-quadcopters (drones) as illustrated in Figure 6. The juggler controls these drones by way of tracked gloves and associated interaction techniques. We presented this work as a poster presentation at IHM 2017 [16]. It has also been demonstrated during a live performance at OARA in Bordeaux on November 23rd, part of the FACTS festival.

7.4. New version of Teegi and its pedagogical potential

Participants: Jeremy Frey, Fabien Lotte and Martin Hachet

Cerebral activity is an intangible physiological process that is difficult to apprehend, especially for children. To overcome this difficulty, Teegi was designed as a new type of educational support. This tangible interface enables children to discover the relationship between brain activity and the functions of the human body.

This year, we have designed a new version of Teegi (see Figure 7. It is 3D printed, and embeds a Raspberry Pi 3 and NiMh batteries (autonomy of approximately 2 hours). A python script on the Raspberry Pi handles the 402 LEDs (Adafruit Neopixel) covering the “head”, which are connected to its GPIO pins. For a smoother display, the light of the LEDs is diffused by a 3mm thick cap made of acrylic glass. Two 8-by-8 white LEDs matrices picture the eyes. The script also commands the servomotors placed in the hands and feet, 4 Dynamixel XL320.

We used this new version of Teegi as a case of study for developing a multi-methods research approach to estimate the pedagogical potential of a tangible interface used in a real-life educational context. Using this methodology, we conducted a user study (N=29) that highlighted the strengths of this interface, both in terms
of its usability and its impact on learning. Moreover, results revealed possible improvements to further increase pedagogical effectiveness. This type of interface, as well as the evaluation method that we propose, contribute to extending our knowledge concerning the pedagogical use of new interactive tools at school.

This work was published at IHM 2017 [22], and the accompanying demo won the best demo award. Teegi was also demonstrated at CHI 2017 [23].

7.5. One Reality

Participants: Joan Sol Roo and Martin Hachet

This project explores the combination of Physical and Virtual Reality through the usage of Mixed Reality. Early explorations involved the usage of Spatial Augmented Reality in combination with Virtual Reality, two technologies with complementary characteristics that evolved separately in the past. Spatial Augmented Reality (SAR) augments the environment using projectors or screens, without the need of user instrumentation. By keeping a single unified frame of reference, it supports social interaction and natural perception of
the space, but the augmentation is limited by physical constraints (e.g., it requires a surface to display information). Immersive head mounted displays on the other hand are not limited by the physical properties of the environment, yet they isolate the user from their environment. We have proposed a unified frame of reference for both SAR and immersive displays, where the users can select the visualization that is best suited for a given task (Figure 8). This enables both asymmetric collaboration between users, and back-and-forths for a single user. These explorations were followed by the combination of additional modalities, in an incremental fashion. This way, one or more users can chose the desired modalities, and immerse themselves as much as the task requires. As a result, the virtual world can be framed in relationship with the physical one.

A preliminary version of this work was presented at 3DUI 2017 [30] where we obtained a best paper - honorable mention- award. An extended version of this work was then presented at UIST 2017 [33].

In order for such systems to succeed, it is required that users are able to create unified mental models out of heterogeneous representations. To better understand how humans perceive hybrid systems as the one described above, we conducted two studies. They focused on the users’ performance on heterogeneous systems (using Spatial Augmented Reality and immersive Virtual Reality displays), and combining viewpoints (egocentric and exocentric). The results show robust estimation capabilities across conditions. This work has been (conditionally) accepted at CHI 18.

Figure 8. One Reality combines the real and virtual worlds

7.6. Collaboration in VR

Participants: Damien Clergeaud and Pascal Guitton

The aerospace industry is no longer composed of local and individual businesses. Due to the complexity of the products (their size, the number of components, the variety of systems and regulation constraints), the design of an aircraft or a launcher involves a considerable number of engineers with various fields of expertise. Furthermore, aerospace companies often have industrial facilities all over the world. In such a complex setting, it is necessary to build virtual experiments that can be shared between different remote sites. Specific problems then arise, particularly in terms of the perception of other immersed users and of interaction tasks involving several immersed users.

We work with Airbus Group in order to design efficient collaborative interaction methods. These collaborative sessions allow multiple sites to be connected within the same virtual experiment and enable experts from different fields to be immersed simultaneously. For instance, if a problem occurs during the final stages of a launcher assembly, it may be necessary to bring together experts on different sites who were involved in
previous steps (initial design, manufacturing processes). In the context of this collaboration, we are working on various projects:

- Design of basic communication tools for the aerospace context.
- Pano: a 360° visualization system that’s facilitate the communication in the case of guiding someone else [19],
- Design of an Annotation System for taking notes in VR [18].

Figure 9. An immersed user has to perform a virtual task in a complex environment. In order to help the user to be fully aware of the VE, another immersed operator may guide him using a Through-The-Lens metaphor.

7.7. Tangible interaction and augmented reality for collaborative learning

Participants: Philippe Giraudieau and Martin Hachet

Part of the e-Fran project e-Tac, we explore approaches based on the hybridization of physical and digital content for mind-mapping activities at schools. Based on the literature in the fields of cognitive science and HCI, we have designed a mixed-reality (MR) interface called Reality-Map (Figure 10. We conducted a pilot study with 11 participants suggesting that learning and manipulating information about the brain and their cognitive functions could be improved by the use of such a MR interface compared to a traditional WIMP interface [45]. We are now extending this approach with the partners of the project to design and develop a new pedagogical tool that will be evaluated in classrooms.

7.8. A model of Mental-Imagery BCI

Participants: Camille Jeunet and Fabien Lotte

Mental-Imagery based Brain-Computer Interfaces (MI-BCIs) enable users to control applications using their brain activity alone, by realising mental imagery tasks. Although promising, MI-BCIs remain barely used outside laboratories, notably due to the difficulties users encounter when attempting to control them. We claim that understanding and improving the user training process could greatly improve users’ MI-BCI control abilities. Yet, to better understand the training process, we need a model of the factors impacting MI-BCI performance. In other words, we need to understand which traits and states impact MI-BCI performance, how these factors interact and how to influence them to improve this performance. Such a model would enable us to design adapted and adaptive training protocols, to guide eurhythmo physiological analyses or design informed classifiers, among others. In this paper we propose a theoretical model of MI-BCI tasks, which is the first step towards the design of this full cognitive and computational model. This work was published in the International BCI conference [46].
Figure 10. Digital and physical objects combined for collaborative learning

Figure 11. A conceptual model of Mental-Imagery BCI user training
7.9. PEANUT - Personalized Emotional Agent for Neurotechnology User Training

Participants: Léa Pillette, Camille Jeunet and Fabien Lotte

Mental-Imagery based Brain-Computer Interfaces (MI-BCI) are neurotechnologies enabling users to control applications using their brain activity alone. Although promising, they are barely used outside laboratories because they are poorly reliable, partly due to inappropriate training protocols. Indeed, it has been shown that tense and non-autonomous users, that is to say those who require the greatest social presence and emotional support, struggle to use MI-BCI. Yet, the importance of such support during MI-BCI training is neglected. Therefore we designed and tested PEANUT, the first Learning Companion providing social presence and emotional support dedicated to the improvement of MI-BCI user-training. PEANUT was designed based on the literature, data analyses and user-studies. Promising results revealed that participants accompanied by PEANUT found the MI-BCI system significantly more usable. This work was published in the International BCI conference [29].

7.10. The Impact of Flow on BCI user training

Participants: Jelena Mladenovic, Jérémy Frey, Manon Bonnet-Save, Fabien Lotte

Major issues in Brain Computer Interfaces (BCIs) include low usability and poor user performance. This paper tackles them by ensuring the users to be in a state of immersion, control and motivation, called state of flow. Indeed, in various disciplines, being in the state of flow was shown to improve performances and learning. Hence, we intended to draw BCI users in a flow state to improve both their subjective experience and their performances. In a Motor Imagery BCI game, we manipulated flow in two ways: 1) by adapting the task difficulty and 2) by using background music. Results showed that the difficulty adaptation induced a higher flow state, however music had no effect. There was a positive correlation between subjective flow scores and offline performance, although the flow factors had no effect (adaptation) or negative effect (music) on online performance. Overall, favoring the flow state seems a promising approach for enhancing users’ satisfaction, although its complexity requires more thorough investigations. This work was published at the international BCI conference [27]

7.11. New Performance metrics to study BCI user training

Participants: Fabien Lotte and Camille Jeunet
While promising for many applications, Electroencephalography (EEG)-based Brain-Computer Interfaces (BCIs) are still scarcely used outside laboratories, due to a poor reliability. It is thus necessary to study and fix this reliability issue. Doing so requires to use appropriate reliability metrics to quantify both signal processing and user learning performances. So far, Classification Accuracy (CA) is the typical metric used for both aspects. However, we argue in this paper that CA is a poor metric to study how well users are learning to use the BCI. Indeed CA is notably unspecific, discrete, training data and classifier dependent, and as such may not always reflect successful EEG pattern self-modulation by the user. We thus propose new performance metrics to specifically measure how distinct and stable the EEG patterns produced by the user are. By re-analyzing EEG data with these metrics, we indeed confirm that CA may hide some learning effects or hide the user inability to self-modulate a given EEG pattern. This was published at the international BCI Conference [25].

7.12. Joint EEG-fMRI Neurofeedback training

Participants: Fabien Lotte

Neurofeedback is a promising tool for brain rehabilitation and peak performance training. Neurofeedback approaches usually rely on a single brain imaging modality such as EEG or fMRI. Combining these modalities for neurofeedback training could allow to provide richer information to the subject and could thus enable him/her to achieve faster and more specific self-regulation. Yet unimodal and multimodal neurofeedback have never been compared before. In the present work, we introduce a simultaneous EEG-fMRI experimental protocol in which participants performed a motor-imagery task in unimodal and bimodal NF conditions. With this protocol we were able to compare for the first time the effects of unimodal EEG-neurofeedback and fMRI-neurofeedback versus bimodal EEG-fMRI-neurofeedback by looking both at EEG and fMRI activations. We also propose a new feedback metaphor for bimodal EEG-fMRI-neurofeedback that integrates both EEG and fMRI signal in a single bi-dimensional feedback (a ball moving in 2D). Such a feedback is intended to relieve the cognitive load of the subject by presenting the bimodal neurofeedback task as a single regulation task instead of two. Additionally, this integrated feedback metaphor gives flexibility on defining a bimodal neurofeedback target. Participants were able to regulate activity in their motor regions in all NF conditions. Moreover, motor activations as revealed by offline fMRI analysis were stronger during EEG-fMRI-neurofeedback than during EEG-neurofeedback. This result suggests that EEG-fMRI-neurofeedback could be more specific or more engaging than EEG-neurofeedback. Our results also suggest that during EEG-fMRI-neurofeedback, participants tended to regulate more the modality that was harder to control. Taken together our results shed first light on the specific mechanisms of bimodal EEG-fMRI-neurofeedback and on its added-value as compared to unimodal EEG-neurofeedback and fMRI-neurofeedback.
This work in collaboration with Inria teams Hybrid, Visage and Athena, was published in the journal Frontiers in Neuroscience [14].

7.13. Robust EEG spatial filters for single trial regression

**Participants:** Fabien Lotte

In the field of Brain-Computer Interfaces (BCI), robust methods for the decoding of continuous brain states are of great interest as new application fields are arising. When capturing brain activity by an electroencephalogram (EEG), the Source Power Comodulation (SPoC) algorithm allows to compute spatial filters for the decoding of a continuous variable. However, dealing with high-dimensional EEG data that suffer from low signal-to-noise ratio, the method reveals instabilities for small training data sets and is prone to overfitting. In this paper, we introduce a framework for applying Tikhonov regularization to the SPoC approach in order to restrict the solution space of filters. Our findings show that an additional trace normalization of the included covariance matrices is a necessary prerequisite to tune the sensitivity of the resulting algorithm. In an offline analysis with data from N=18 subjects, the introduced trace normalized and Tihonov regularized SPoC variant (NTR-SPoC) outperforms the standard SPoC method for the majority of individuals. With this proof-of-concept study, a generalizable regularization framework for SPoC has been established which allows to implement a variety of different regularization strategies in the future. This work in collaboration with Freiburg University, Germany, was published at the international BCI Conference [26].


**Participants:** Fabien Lotte

SensoriMotor Rhythm (SMR)-based Brain-Computer Interfaces (BCI) are among the most used ElectroEncephaloGraphy (EEG) BCI systems. However, such systems have low performance and many of their users are “non-responders”. There is thus a need to understand the limitations of current SMR-BCI and to improve them. Many of them use machine learning. They are typically calibrated on EEG signals collected while the users are performing Motor Imagery (MI), i.e., imagining limb movements. Once calibrated, they also use MI as control strategy. However, for many first time users of SMR-BCI, performing MI is new and difficult, and they may be unable to perform clear MI. Thus, using MI for calibration may result in suboptimal EEG features and corresponding real-time feedback. Therefore, we aim at elucidating whether MI tasks are the best motor tasks to use for calibration and control in SMR-BCI. To do so, we collected EEG signals from subjects instructed to perform four different motor tasks and a rest task, for multiple trials. In particular, subjects have to 1) execute real feet movements; 2) imagine feet movements (walking); 3) observe feet movements (walking), in a first person view and 4) observe feet movements while imagining them at the same time. Preliminary results revealed that for some subjects, calibrating EEG spatial filters on real motor movements can lead to better performances with an MI-BCI than calibrating them on MI tasks. This thus warrant further investigation into the calibration tasks in SMR-BCI. This preliminary work, in collaboration with RIKEN Brain Science Institute in Japan, was presented as a poster at RTFIN 2017 [48].

7.15. A review of Rapid Serial Visualization Protocol-based BCI

**Participants:** Fabien Lotte

Rapid serial visual presentation (RSVP) combined with the detection of event related brain responses facilitates the selection of relevant information contained in a stream of images presented rapidly to a human. Event related potentials (ERPs), measured non-invasively with electroencephalography (EEG), can be associated with infrequent target stimuli(images) in groups of images, potentially providing an interface for human-machine symbiosis, where humans can interact and interface with a computer without moving and which may offer faster image sorting than scenarios where humans are expected to physically react when a target image is detected. Certain features of the human visual system impact on the success of the RSVP paradigm. Pre-attentive processing supports the identification of target information 100ms following information presentation. This paper presents a comprehensive review and evaluation of research in the broad
field of RSVP-based brain-computer interfaces (BCIs). Applications that use RSVP-based BCIs are classified based on the operation mode whilst protocol design considerations are critiqued. Guidelines for using the RSVP-based BCI paradigms are defined and discussed, with a view to further standardization of methods and experimental evidence gathering to support the use of RSVP-based BCIs in practice. This review in collaboration with Ulster University, UK, was published in Journal of Neural Engineering [13].

7.16. Active Inference-based design of adaptive P300-Speller BCIs

**Participants:** Jelena Mladenovic, Fabien Lotte

Recent developments in computational neuroscience gave rise to an efficient generic framework to implement both optimal perceptual (Bayesian) inference and choice behaviour. This framework named Active Inference rests on minimizing free energy or surprise [3]. We suggest it could be used to implement efficient adaptive Brain-Computer Interfaces (BCIs). We briefly illustrate it on a simulated P300-speller task. This work in collaboration with Inserm Lyon, was published in the first Neuro Adaptive Technology conference [28].

7.17. BCI Handbook

**Participants:** Fabien Lotte

Together with Chang S Nam (USA) and Anton Nijholt (Netherlands/Malaysia), we edited an Handbook of BCI technologies [41]. This handbook is a valuable resource to anyone involved with improvement of people’s lives by replacing, restoring, supplementing and improving motor action, and understanding the neural bases of such functions. While there are several other resources available, there is no handbook such as this one. This handbook addresses the recent and rapid changes in the field of braincomputer interfaces (BCIs). Due to these changes interest in BCI has grown enormously, including interest from computer science researchers with a background in computational intelligence, human-computer interaction, and researchers in entertainment technology.

7.18. Augmented Reality Maps for Visually Impaired People

**Participants:** Anke Brock

VISTE builds on the previous development of the GEOTHNK platform (Kavouras et al., 2016). The VISTE framework and associated resources and tools focus on collaborative learning of spatial concepts and skills for sighted and VI students to foster inclusion within mainstream education. VISTE will empower students with VI to acquire spatial skills through specially designed learning activities as well as through an augmented reality prototype. At Inria Bordeaux, we have designed and implemented an augmented reality prototype that can be used as spatial thinking training tool in special education schools. It makes use of the PapARt technology, an OpenSource augmented reality framework 0. Current low-tech Orientation & Mobility (O&M) tools for visually impaired people, e.g. tactile maps, possess limitations. Interactive accessible maps have been developed to overcome these 0. However, most of them are limited to exploration of existing maps, and have remained in laboratories. Using a participatory design approach, we have worked closely with 15 visually impaired students and 3 O&M instructors over 6 months. We iteratively designed and developed an augmented reality map destined at use in O&M classes in special education centers. This prototype combines projection, audio output and use of tactile tokens, and thus allows both map exploration and construction by low vision and blind people. Our user study demonstrated that all students were able to successfully use the prototype, and showed a high user satisfaction. A second phase with 22 international special education teachers allowed us to gain more qualitative insights. This work shows that augmented reality has potential for improving the access to education for visually impaired people. A publication about this map prototype and the user study has been (conditionally) accepted at CHI’18 0 Learn more about VISTE project: http://visteproject.eu/https://team.inria.fr/potioc/viste-empowering-spatial-thinking-of-students-with-visual-impairment/

0Laviole & Hachet, 2012
0Ducasse et al., 2018
7.19. Accessibility of e-learning systems

Participants: Pierre-Antoine Cinquin and Pascal Guitton

New digital teaching systems such as MOOCs are taking an increasingly important place in current teaching practices. Unfortunately, accessibility for people with disabilities is often forgotten, which excludes them, particularly those with cognitive impairments for whom accessibility standards are fare from being established. This is truly unfortunate as the interest of using these specialized practices for this audience is scientifically proven.

To overcome these limitations, we propose new design principles based on knowledge in the areas of accessibility (Ability-based Design and Universal Design), digital pedagogy (Instruction Design with functionalities that reduce the cognitive load: navigation by concept, slowing of the flow...), specialized pedagogy (Universal Design for Learning, eg, automatic note-taking, and Self Determination Theory, e.g., configuration of the interface according to users needs and preferences) and psycheducational interventions (eg, support the joint teacher-learner attention), but also through a participatory design approach involving students with disabilities and experts in the field of disability. From these framework, we have designed interaction features which have been implemented in a specific MOOC player called Aïana. Moreover, we have produced a MOOC on digital accessibility which is published on the national MOOC platform (FUN) using Aïana (2 sessions in 2016 and 2017) https://mooc-francophone.com/cours/mooc-accessibilite-numerique/.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Interactive Collaboration in Virtual Reality for Aerospace Scenarii:
Duration: 2014-2017
PhD Thesis of Damien Clergeaud
Partners: Airbus Group
Local coordinator: Pascal Guitton
The Airbus company regularly uses virtual reality for design, manufacturing and maintenance. We work with them on collaborative interaction in order to enable an efficient collaboration between operators immersed in the virtual environment from remote locations and with heterogeneous equipment. More precisely, we have developed tools to point and manipulate objects, to remotely visualize the virtual environment, to be aware of remote manipulations and to describe tools and components trajectories.

9. Partnerships and Cooperations

9.1. Regional Initiatives

Introspectibles - Collaborative research project:
Funding: Région Aquitaine
Duration: 2017-2018
Local coordinator: Martin Hachet
Partners: ULLO,
Following our work with the Introspectibles (Teegi, TOBE, Inner Garden), we are currently working with the ULLO company to bring these new interfaces to healthcare centers.

HOBIT - Maturation project:
Funding: Aquitaine Science Transfer
Duration: 2017-2018
Local coordinator: Martin Hachet
Partners: Université de Bordeaux
We are currently moving our platform HOBIT from his lab state to a commercial product.

Km 2.0 - Arts an Sciences program:
Funding: Idex Université Bordeaux
Duration: 2017-2018
Local coordinator: Martin Hachet
Partners: Léna D’Azy
We work with Cécile Léna for creating artistic installations based on interactive projection. See http://www.facts-bordeaux.fr/RESIDENCES/KM-2.0

Telekinetik juggling - Arts an Sciences program:
Funding: Idex Université Bordeaux
Duration: 2017-2018
Local coordinator: Martin Hachet
Partners: Le Cirque Inachevé
We work with Antoine Cléé from Cirque Inachevé for the design of an interactive environment where the artist will be able to juggle with zero gravity objects. The artist wear gloves, and interact with mini-drones supporting balls. See http://www.facts-bordeaux.fr/RESIDENCES/Jonglerie-telekinetique
Neuroperf:
Funding: Idex Université Bordeaux
Duration: 2017-2019
Coordinator: Jean-Arthur Micoulaud Franci
Local coordinator: Fabien Lotte
Partners: SANPSY - Potioc
This project aims at studying EEG-based Neurofeedback to reduce fatigue symptoms in sleep-deprived individuals. See [http://brain.labex.u-bordeaux.fr/Actualites/Selection-projets-recherche-Clinique-2017-i5064.html](http://brain.labex.u-bordeaux.fr/Actualites/Selection-projets-recherche-Clinique-2017-i5064.html)

9.2. National Initiatives

eTAC: Tangible and Augmented Interfaces for Collaborative Learning:
Funding: EFRAN
Duration: 2017-2021
Coordinator: Université de Lorraine
Local coordinator: Martin Hachet
Partners: Université de Lorraine, Inria, ESPE, Canopé, OpenEdge,
the e-TAC project proposes to investigate the potential of technologies "beyond the mouse" in order to promote collaborative learning in a school context. In particular, we will explore augmented reality and tangible interfaces, which supports active learning and favors social interaction.

ANR Rebel:
Duration: 2016-2019
Coordinator: Fabien Lotte
Funding: ANR Jeune Chercheur Jeune Chercheuse Project
Partners: Disabilities and Nervous Systems Laboratory Bordeaux
Brain-Computer Interfaces (BCI) are communication systems that enable their users to send commands to computers through brain activity only. While BCI are very promising for assistive technologies or human-computer interaction (HCI), they are barely used outside laboratories, due to a poor reliability. Designing a BCI requires 1) its user to learn to produce distinct brain activity patterns and 2) the machine to recognize these patterns using signal processing. Most research efforts focused on signal processing. However, BCI user training is as essential but is only scarcely studied and based on heuristics that do not satisfy human learning principles. Thus, currently poor BCI reliability is probably due to suboptimal user training. Thus, we propose to create a new generation of BCI that apply human learning principles in their design to ensure the users can learn high quality control skills, hence making BCI reliable. This could change HCI as BCI have promised but failed to do so far.

ANR Project ISAR:
Duration: 2014-2017
Coordinator: Martin Hachet
Partners: LIG-CNRS (Grenoble), Diotasoft (Paris)
Acronym: Interaction en Réalité Augmentée Spatiale / Interacting with Spatial Augmented Reality
The ISAR project (Interaction with Spatial Augmented Reality) focuses on the design, implementation, and evaluation of new paradigms to improve interaction with the digital world when digital content is directly projected onto physical objects. It opens new perspectives for exciting tomorrow’s applications, beyond traditional screen-based applications.
website: [https://team.inria.fr/potioc/scientific-subjects/papart/](https://team.inria.fr/potioc/scientific-subjects/papart/)
**Inria Project Lab BCI-LIFT:**

Duration: 2015-2018

Partners: Inria team Athena (Inria Sophia-Antipolis), Inria team Hybrid (Inria Rennes), Inria team Neurosys (Inria Nancy), LITIS (Université de Rouen), Inria team DEMAR (Inria Sophia-Antipolis), Inria team MINT (Inria Lille), DyCOG (INSERM Lyon)

Coordinator: Maureen Clerc (Inria Sophia Antipolis)

Local coordinator: Fabien Lotte

The aim is to reach a next generation of non-invasive Brain-Computer Interfaces (BCI), more specifically BCI that are easier to appropriate, more efficient, and suit a larger number of people. With this concern of usability as our driving objective, we will build non-invasive systems that benefit from advanced signal processing and machine learning methods, from smart interface design, and where the user immediately receives supportive feedback. What drives this project is the concern that a substantial proportion of human participants is currently categorized “BCI-illiterate” because of their apparent inability to communicate through BCI. Through this project we aim at making it easier for people to learn to use the BCI, by implementing appropriate machine learning methods and developing user training scenarios.


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**9.3. European Initiatives**

**9.3.1. FP7 & H2020 Projects**

Program: ERC Starting Grant

Project acronym: BrainConquest

Project title: Boosting Brain-Computer Communication with High Quality User Training

Duration: 07/2017-06/2022

Coordinator: Fabien Lotte

Abstract: Brain-Computer Interfaces (BCIs) are communication systems that enable users to send commands to computers through brain signals only, by measuring and processing these signals. Making computer control possible without any physical activity, BCIs have promised to revolutionize many application areas, notably assistive technologies, e.g., for wheelchair control, and man-machine interaction. Despite this promising potential, BCIs are still barely used outside laboratories, due to their current poor reliability. For instance, BCIs only using two imagined hand movements as mental commands decode, on average, less than 80% of these commands correctly, while 10 to 30% of users cannot control a BCI at all. A BCI should be considered a co-adaptive communication system: its users learn to encode commands in their brain signals (with mental imagery) that the machine learns to decode using signal processing. Most research efforts so far have been dedicated to decoding the commands. However, BCI control is a skill that users have to learn too. Unfortunately how BCI users learn to encode the commands is essential but is barely studied, i.e., fundamental knowledge about how users learn BCI control is lacking. Moreover standard training approaches are only based on heuristics, without satisfying human learning principles. Thus, poor BCI reliability is probably largely due to highly suboptimal user training. In order to obtain a truly reliable BCI we need to completely redefine user training approaches. To do so, I propose to study and statistically model how users learn to encode BCI commands. Then, based on human learning principles and this model, I propose to create a new generation of BCIs which ensure that users learn how to successfully encode commands with high signal-to-noise ratio in their brain signals, hence making BCIs dramatically more reliable. Such a reliable BCI could positively change man-machine interaction as BCIs have promised but failed to do so far.
9.3.2. Collaborations in European Programs, Except FP7 & H2020

• Program: DGA-DSTL Project
  Project title: Assessing and Optimising Human-Machine Symbiosis through Neural signals for Big Data Analytics
  Duration: 2014-2018
  Coordinator: Damien Coyle and Fabien Lotte
  Partners: Ulster University, UK, Potioc, France
  Abstract: This project objective is to design new tools for Big Data analysis, and in particular visual analytics tools that tap onto human cognitive skills as well as on Brain-Computer Interfaces. The goal is to enable the user to identify and select relevant information much faster than what can be achieved by using automatic tools or traditional human-computer interfaces. More specifically, this project will aim at identifying in a passive way various mental states (e.g., different kinds of attention, mental workload, relevant stimulus perception, etc.) in order to optimize the display, the arrangement of the selection of relevant information.

• Program: ERASMUS+
  Project acronym: VISTE
  Project title: Empowering spatial thinking of students with visual impairment
  Duration: 2016-2019
  Coordinator: National Technical University of Athens (Greece)
  Local coordinator: Anke Brock
  Other partners: Intrasoft International SA (Greece), Casa Copolui Didatic Cluj (Romania), Liceul Special pentru Deficienti de Vedere Cluj-Napoca (Romania), Eidiko Dimotiko Sxolio Tiflon Kallitheas (Greece)
  Abstract: VISTE addresses inclusion and diversity through an innovative, integrated approach for enhancing spatial thinking focusing on the unique needs of students with blindness or visual impairment. However, since spatial thinking is a critical competence for all students, the VISTE framework and associated resources and tools will focus on cultivating this competence through collaborative learning of spatial concepts and skills both for sighted and visually impaired students to foster inclusion within mainstream education. The VISTE project will introduce innovative educational practices for empowering students with blindness or visual impairment with spatial skills through specially designed educational scenarios and learning activities as well as through a spatial augmented reality prototype to support collaborative learning of spatial skills both for sighted and visually impaired students.

9.3.3. Collaborations with Major European Organizations

Partner 1: Univ. Freiburg, Brain State Decoding Laboratory (M. Tangermann), Germany
  Topic 1: robust EEG spatial filters for single trial regression

Partner 2: TU Graz, Neural Engineering lab (R. Scherer), Austria
  Topic 2: BCI pitfalls, negative results in BCI, guidelines for BCI design

Partner 3: EPFL, Defitech Foundation Chair in Brain-machine Interface (R. Chavarriaga), Switzerland
  Topic 3: BCI pitfalls, negative results in BCI

Partner 4: Oldenbourg University, Neuropsychology department (S. Debener, C. Zich), Germany
  Topic 4: guidelines for BCI design
9.4. International Initiatives

9.4.1. Inria International Labs

9.4.1.1. Other IIL projects

Presentation of Potioc research activities during the annual Inria-EPFL Workshop (Session MOOCS & e-learning)

9.4.2. Inria International Partners

9.4.2.1. Informal International Partners

Partner: Université du Québec à Montréal, Institut des Sciences Cognitives (R. N’Kambou), Montreal, Canada
Topic: Learning companions for Brain-Computer Interfaces
Partner: North Carolina State University (Chang S. Nam), USA
Topic: Handbook of Brain-Computer Interfaces

9.4.3. Participation in Other International Programs

Partner: Flowers & Potioc teams, Inria Bordeaux, University of Waterloo, Canada
Funding: Univ. Bordeaux/Univ Waterloo joint grant call for project
Date: 2017-2018
Topic: Designing for Curiosity in Physical Spaces

9.5. International Research Visitors

9.5.1. Visits to International Teams

9.5.1.1. Research Stays Abroad

3 Members of team Potioc spend several months at the RIKEN Brain Science Institute (BSI), Cichocki’s advanced brain signal processing laboratory, Wakoshi, Japan.

- Fabien Lotte: 10 months in total, with the JSPS (Japan Society for the Promotion of Science) Invitation fellowship program
- Léa Pillette: 6 months in total, funded by the RIKEN BSI
- Aurélien Appriou: 3 months in total, funded by the RIKEN BSI

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- EduIHM, Workshop at IHM 2017, Martin Hachet
- “Kick-off conference of CORTICO, the French BCI association”, Paris, France, January 2017, Fabien Lotte
10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees
- Program Chair IHM 2017, Martin Hachet

10.1.2.2. Member of the Conference Program Committees
- ACM CHI Conference, 2018, Anke Brock
- ACM ASSETS Conference, 2017, Anke Brock
- Late Breaking Work Committee ACM CHI Conference, 2017, Anke Brock
- Augmented Human Conference (AH), 2018, Fabien Lotte
- Eurographics STA,R 2017, Martin Hachet
- IEEE VR, 2017, Martin Hachet
- 7th International Brain-Computer Interface Conference, 2017, Fabien Lotte
- Neuroadaptive Technology conference (NAT), 2017, Fabien Lotte
- Symbiotic, 2017, Fabien Lotte

10.1.2.3. Reviewer
- ACM CHI 2018, Pascal Guitton, Fabien Lotte, Joan Sol Roo
- ACM ISS 2017, Joan Sol Roo
- ACM CHI-Play 2017, Joan Sol Roo
- ACM UIST 2017, Fabien Lotte
- Augmented Human Conference (AH), 2018, Fabien Lotte, Jelena Mladenovic
- Haptics Symposium 2018, Anke Brock
- ICASSP 2018, Fabien Lotte
- IEEE VR 2018, Joan Sol Roo
- 7th International Brain-Computer Interface Conference, 2017, Fabien Lotte
- JJ-ICON 2017, Fabien Lotte
- MobileHCI 2017, Anke Brock
- Symbiotic 2017, Fabien Lotte

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards
- Special Issue Chair TACCESS ACM ASSETS Conference, 2017, Anke Brock
- Member of the Editorial board of Journal of Neural Engineering, Fabien Lotte
- Member of the Editorial Board (Associate Editor) of the Brain-Computer Interface journal, Fabien Lotte
- Review Editor for the Frontiers in Human-Media Interaction journal, Fabien Lotte
- Review Editor for the Frontiers in Neuroprosthetics journal, Fabien Lotte
- Guest Editor, Frontiers in Neurosciences on “Detection and Estimation of Working Memory States and Cognitive Functions Based on Neurophysiological Measures”, 2017, Fabien Lotte

10.1.3.2. Reviewer - Reviewing Activities
- ACM Transactions on Computer-Humans Interactions (TOCHI), Fabien Lotte
- BioMed Research International, Fabien Lotte
- Frontiers in Human Neurosciences, Fabien Lotte
- IEEE Access, Fabien Lotte
- IEEE Transactions on Biomedical Engineering, Fabien Lotte
• IEEE Transactions on Human-Machine Systems, Fabien Lotte
• International Journal of Human-Computer Studies, Fabien Lotte
• Journal of Accessibility and Design for All (JACCESS), Anke Brock
• Journal of Neural Engineering, Fabien Lotte
• Nature Scientific Reports, Fabien Lotte
• PLOS One, Fabien Lotte
• Transactions on Haptics, Anke Brock

10.1.4. Invited Talks

• Which feedback should be given to maximize Brain-Computer Interface training, 2nd National Day about Neurofeedback at ESPCI school in Paris, France, Jan. 2017, Léa Pillette
• The impact of flow on BCI neurofeedback training, 2nd National Day about Neurofeedback at ESPCI school in Paris, France, Jan. 2017, Jelena Mladenovic
• Engagement des publics et genre, Séminaire Projet RRI-Practice, CEA Saclay, Feb. 2017, Pascal Guitton
• Comment apprendre à contrôler un ordinateur avec son activité cérébrale ? Le projet BrainConquest, Journée 10 ans ERC - 50 ans Inria, Paris, March 2017, Fabien Lotte
• Art and Sciences at Potioc, Ministry of Culture, Paris, March 2017, Martin Hachet
• Multisensory Maps for Visually Impaired People, Robotics, Brain and Cognitive Sciences dept, Italian Institute of Technology, Genova, Italy, APRil 2017, Anke Brock
• Designing for Accessibility, University Bordeaux, OpenCare Project Meeting (H2020), June 2017, Anke Brock
• L’éthique en Sciences du numérique, Ecole du Management Inria, Paris, June 2017, Pascal Guitton
• Creating, learning, and meditating; a trip in tangible hybrid spaces, ETIS, Luxembourg, June 2017, Martin Hachet
• Augmented reality & tangible interaction for accessibility, University Stuttgart, HCI Lab, July 2017, Anke Brock
• Understanding and improving BCI user training to boost brain-computer communications, International Graz Brain-Computer Interfaces Conference, opening Keynote, Graz, Austria, Sep. 2017, Fabien Lotte
• Brain-Computer Interfaces technologies for the benefit of all: Neuroergonomics and Neuroeducation, Tokyo University of Agriculture and Technology (TUAT), Tokyo, Japan, Oct. 2017, Fabien Lotte
• Brain-Computer Interfaces: design, user training and new applications, Japanese French Laboratory for Informatics (JFLI), Tokyo University, Tokyo, Japan, Oct. 2017, Fabien Lotte
• L’accessibilité des systèmes numériques d’enseignement, GT Handicap, FCS Paris-Saclay, Nov. 2017, Pascal Guitton
• Interactive projection and 3D gestures for Artistic performances, OARA, Bordeaux, Nov. 2017, Martin Hachet
• Combining machine learning and psychology to design usable Brain-Computer Interfaces, RIKEN Advanced Intelligence Project, Tokyo, Japan, Dec. 2017, Fabien Lotte

10.1.5. Scientific Expertise

• Reviewer for the Millennium Science Initiative 2017, Chile, Fabien Lotte
• Membre du comité ANR CE33 (Interaction, Robotics) 2017, Fabien Lotte
• Member of Inria Cellule de veille et de prospective, Pascal Guitton
• Reviews of projects: ANR, DFG, Crédit Impot Recherche (Ministère de la recherche), Anke Brock, Martin Hachet
• Member of COSAE, scientific board of SCRIME, Martin Hachet
• Member of the scientific board of ULLO, Martin Hachet, Fabien Lotte

10.1.6. Research Administration
• Representative of Inria at NEM (New European Media), Fabien Lotte
• Member of Commission de recrutement des Inspecteurs Généraux de l’Education Nationale (IGEN), Pascal Guitton
• Member of Comité de Pilotage de Software Heritage, Pascal Guitton
• Femmes & Sciences Deputy Board Member, Anke Brock
• Member of Inria Ethical Committee (COERLE), Pascal Guitton
• Member of Inria Comité Parité et Egalité, Anke Brock & Pascal Guitton
• Responsible of Inria RA2020 Committee (new annual Activity Report), Pascal Guitton
• Member of Inria International Chairs Committee, Pascal Guitton
• Member of Comité de sélection Professeur d’informatique, Université de Rennes, Pascal Guitton
• Jury member for the competitive selection - Young graduate scientist (Chargé de Recherche 2) at Inria Bordeaux (2017), Anke Brock
• Jury member for an Assistant Professorship (MCF section CNU 63, “Photonics and digital sciences”) at Institut Optique / Université Paris-Sud, Anke Brock
• Jury member for the competitive selection Research scientist (CR 2) at Inria Bordeaux, Anke Brock
• Member of Bureau du comité des projets, Inria Bordeaux Sud-Ouest, Martin Hachet
• Member of Comité de Dévelopement Technologique (CDT), Inria Bordeaux Sud-Ouest, Fabien Lotte
• Member of Comité Jeunes Chercheurs at Inria Bordeaux Sud-Ouest, Anke Brock
• Member of Comité de Pilotage Responsabilité Sociétale de l’Université, Université de Bordeaux, Pascal Guitton

10.2. Teaching - Supervision - Juries
10.2.1. Teaching
Licence Pierre-Antoine Cinquin, Assistive technologies for cognition, CM, 3h, 2nd year Institut de formation en ergothérapie, Bordeaux, France
Master: Pascal Guitton, Virtual and Augmented Realities, CM, 36h eqtd, M2 Computer Science, University of Bordeaux, France
Master: Pascal Guitton, Digital accessibility, CM, 12h eqtd, M1 Cognitive Science, University of Bordeaux, France
Master: Pascal Guitton, Assistive technologies, CM, 30h eqtd, M2 Cognitive Science, University of Bordeaux, France
Master: Martin Hachet, Virtual Reality and 3D Interaction, CM, 12h eqtd, M2 Cognitive Science, University of Bordeaux, France
Master: Martin Hachet, Interaction and Ergonomics, CM-TD, 8h eqtd, 3rd year (M2), Enseirb, Bordeaux, France
Master: Fabien Lotte, Brain-Computer Interfaces, CM, 2h, M2 Neuroergonomics & Human Factors International Master, ISAE, Toulouse, France
Master: Léa Pillette, Virtual Reality and 3D Interaction, CM, 5h eqtd, M2 Cognitive Science, University of Bordeaux, France
Master: Léa Pillette, Knowledge and Representations, TD, 54h, 1ère année, Ecole Nationale Supérieure de Cognitique, INP, Bordeaux, France

**E-learning**

MOOC : Pascal Guitton & Hélène Sauzéon, Accessibilité numérique, 5 semaines, Plate-forme France Université Numérique (FUN), Inria, 2ème session (1900 inscrits)

### 10.2.2. Supervision

**PhD:** Lorraine Perronnet, Combing EEG and fMRI for Neurofeedback, Université de Rennes, Sep. 2017, Anatole Lécuyer, Christian Barillot, Maureen Clerc & Fabien Lotte

**PhD:** Damien Clergeaud, Collaborative interaction for aerospace scenarios, Oct. 2017, Pascal Guitton

**PhD:** Joan Sol Roo, One Reality, Augmenting the Human Experience through the Combination of Physical and Digital Worlds, Dec. 2017, Martin Hachet

**PhD in progress:** Stephanie Lees, Ulster University, UK, Assessing and Optimising Human-Machine Symbiosis through Neural signals for Big Data Analytics, since Feb. 2014, Damien Coyle, Fabien Lotte, Paul McCullagh and Liam Maguire

**PhD in progress:** Jelena Mladenovic, BCI user modelling for adaptive BCI training and operation, since Jan. 2016, Fabien Lotte & with Jérémie Mattout

**PhD in progress:** Pierre-Antoine Cinquin, Design and Experimental Validation of Accessible E-learning systems for people with cognitive disabilities, since Sept. 2016, Pascal Guitton & Hélène Sauzéon

**PhD in progress:** Léa Pillette, Redefining Formative Feedback in Brain-Computer Interface User Training, since Oct. 2016, Fabien Lotte & Bernard N’Kaoua

**PhD in progress:** Aurélien Appriou, Estimating learning-related mental states from EEG signals, since Oct. 2017, Fabien Lotte

**PhD in progress:** Philippe Giraudcne, One Reality, Augmented Reality and Tangible Interaction to support Collaborative Learning, since Oct. 2017, Martin Hachet

**PhD in progress:** Stephanie Rey, Design and evaluation of a tool for personalized museum visits, Bourse CIFRE with Berger-Levrault, joint supervision by Anke Brock & Nadine Couture

**PhD in progress:** Rajkumar Darbar, Actuated Tangible User Interfaces, since Dec. 2017, Martin Hachet

### 10.2.3. Juries

- PhD (Reviewer): Paul Issartel, Université Paris Sud, Saclay, 2017 April 3rd, Martin Hachet
- PhD (Reviewer): Mariacarla Memeo, University of Genova and Italian Institute of Technology, April 2017, Anke Brock
- PhD (Reviewer): Jean-Baptiste Barreau, INSA Rennes, 2017 July 10th, Pascal Guitton
- PhD (Reviewer): Kireth Dhindsa, McMaster University, Canada, 2017 Aug., Fabien Lotte
- PhD (Reviewer): Lonni Besançon, Université Paris Sud, Saclay, 2017 Dec. 14th, Martin Hachet
- PhD (Jury member): Cecilia Lindig-Leon, University of Lorraine, France, Jan. 2017, Fabien Lotte
- PhD (Jury member): Philippe Roussille, Université Toulouse 3 (JIRIT), Jan. 2017, Anke Brock
- PhD (Jury member): Sarah Buchanan, University of Central Florida, USA, April 7th, Martin Hachet
- PhD (comité de suivi): Fanny Grosselin, UPMC / ICM / MyBrain technologies, France, 2017, Fabien Lotte

### 10.3. Popularization

**Duties**

- Member of the Editorial board of Blog Binaire - Le Monde, Pascal Guitton
Teaching and Education
- Participation à la création du MOOC Informatique et Création Numérique, Plate-forme FUN, Anke Brock & Pascal Guitton, https://www.fun-mooc.fr/courses/inria/41014/session01/about

Talks and Hands-on
- Collaborer avec la réalité virtuelle, Pint of Sciences, Bordeaux, May 14th, Damien Clergeaud
- Demonstration of VISTE project at Colloque Robotique et Éducation 2017, Bordeaux, July 2017, Anke Brock & Jérémy Albouys
- Demonstration and presentation of VISTE project at Fête de la science, Oct 2017, Jérémy Albouys
- Demonstration and presentation of VISTE project at Nuits des chercheurs at Cap Sciences, Oct. 2017, Jérémy Albouys
- Collaborative Interaction in Virtual Reality, Airbus PhD’s Days, Saint Médard en Jalles, Nov. 8th, Damien Clergeaud
- La Table de Shanghai, Open Lab FACTS Festival, Nov. 14-25th
- Organization of an Hackathon on Cognitive Science and Artificial Intelligence at Bordeaux, Dec 9-10th, Philippe Giraudeau
- Interview, Martin Hachet, Inriality, https://www.inriality.fr/culture-loisirs/se-divertir-en-2067/
- Interview, Martin Hachet, RFI - autour de la question, http://www.rfi.fr/emission/20171113-comment-imaginer-notre-futur
- Interview, Martin Hachet, Libération, http://next.liberation.fr/musique/2017/01/27/un-nouveau-chant-de-vision_1544507

Popularizing inside Inria
- Comment favoriser l’accessibilité numérique, Unithé ou Café, Bordeaux, April 6th, Pascal Guitton
- Teegi, 50th anniversary Inria, Nov 7-8, Paris, Philippe Giraudeau, Martin Hachet

Written, Oral or Video Content
- “Fabien Lotte about his goal to improve BCI usability”, g.tec medical engineering blog, http://blog.gtec.at/interview-fabien-lotte/, 2017
- Interview about VISTE project for LUDOVIAMAGAZINE : https://www.youtube.com/watch?v=Hdw5O0myifY, Anke Brock

11. Bibliography

Major publications by the team in recent years


Publications of the year

**Articles in International Peer-Reviewed Journal**


International Conferences with Proceedings


[17] Best Paper


[24] **Best Paper**

[25] F. LOTTE, C. JEUNET: Online classification accuracy is a poor metric to study mental imagery-based bci user learning: an experimental demonstration and new metrics , in "7th International BCI Conference", Graz, Austria, September 2017, https://hal.archives-ouvertes.fr/hal-01519478.


[30] **Best Paper**


[32] **Best Paper**


Conferences without Proceedings


Scientific Books (or Scientific Book chapters)


Patents and standards


Other Publications


Project-Team REALOPT

Reformulations based algorithms for Combinatorial Optimization

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB), Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Optimization, machine learning and statistical methods
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Project-Team REALOPT

Creation of the Project-Team: 2009 January 01

Keywords:

**Computer Science and Digital Science:**
- A8.1. - Discrete mathematics, combinatorics
- A8.2. - Optimization
- A8.7. - Graph theory

**Other Research Topics and Application Domains:**
- B6.5. - Information systems

1. Personnel

**Research Scientists**
Olivier Beaumont [Inria, Senior Researcher, HDR]
Lionel Eyraud-Dubois [Inria, Researcher]
Vitor Nesello [ADERA, temporary Researcher, from Sep 2017, part-time]
Ruslan Sadykov [Inria, Researcher]

**Faculty Members**
Francois Vanderbeck [Team leader, Univ of Bordeaux, Professor, HDR]
Francois Clautiaux [Univ of Bordeaux, Professor, HDR]
Boris Detienne [Univ of Bordeaux Associate Professor]
Arnaud Pecher [Univ of Bordeaux, Professor, HDR]
Pierre Pesneau [Univ of Bordeaux, Associate Professor]

**External Collaborators**
Cedric Joncour [Univ Du Havre, Assistant Prof]
Sophie Michel [Univ Du Havre, Assistant Prof]
Walid Klibi [Kedge Business School, Bordeaux, Assistant Prof]
Gautier Stauffer [Institut polytechnique de Grenoble, Professor]
Alexis Toullat [Ertus Consulting]

**Technical Staff**
Adeline Fonseca [Inria, from Sep 2017]
Guillaume Marques [Univ, until Aug 2017]
Issam Tahiri [Inria]

**PhD Students**
Thomas Bellitto [ENS]
Imen Ben Mohamed [Kedge Business School, Bordeaux]
Mohamed Benkirane [Cifre SNCF]
Rodolphe Griset [Cifre EDF]
Gael Guillot [Univ de Bordeaux, from Nov 2017]
Jeremy Guillot [Univ of Bordeaux, ATER]
Thomas Lambert [ENS Lyon, until Aug 2017]
Guillaume Marques [Univ of Bordeaux, from Sep 2017]
Quentin Viaud [Cifre Saint-Gobain]

**Post-Doctoral Fellows**
Ayse Nur Arslan [Inria]
2. Overall Objectives

2.1. Overall Objectives

Quantitative modeling is routinely used in both industry and administration to design and operate transporta-
tion, distribution, or production systems. Optimization concerns every stage of the decision-making process: long term investment budgeting and activity planning, tactical management of scarce resources, or the control of day-to-day operations. In many optimization problems that arise in decision support applications the most important decisions (control variables) are discrete in nature: such as on/off decision to buy, to invest, to hire, to send a vehicle, to allocate resources, to decide on precedence in operation planning, or to install a connection in network design. Such **combinatorial optimization** problems can be modeled as linear or nonlinear programs with integer decision variables and extra variables to deal with continuous adjustments. The most widely used modeling tool consists in defining the feasible decision set using linear inequalities with a mix of integer and continuous variables, so-called Mixed Integer Programs (MIP), which already allow a fair description of reality and are also well-suited for global optimization. The solution of such models is essentially based on enumeration techniques and is notoriously difficult given the huge size of the solution space.

Commercial solvers have made significant progress but remain quickly overwhelmed beyond a certain problem size. A key to further progress is the development of better problem formulations that provide strong continuous approximations and hence help to prune the enumerative solution scheme. Effective solution schemes are a complex blend of techniques: cutting planes to better approximate the convex hull of feasible (integer) solutions, extended reformulations (combinatorial relations can be formulated better with extra variables), constraint programming to actively reduce the solution domain through logical implications along variable fixing based on reduced cost, Lagrangian decomposition methods to produce powerful relaxations, and Bender’s decomposition to project the formulation, reducing the problem to the important decision variables, and to implement multi-level programming that models a hierarchy of decision levels or recourse decision in the case of data adjustment, primal heuristics and meta-heuristics (greedy, local improvement, or randomized partial search procedures) to produce good candidates at all stage of the solution process, and branch-and-bound or dynamic programming enumeration schemes to find a global optimum, with specific strong strategies for the selection on the sequence of fixings. The real challenge is to integrate the most efficient methods in one global system so as to prune what is essentially an enumeration based solution technique. The progress are measured in terms of the large scale of input data that can now be solved, the integration of many decision levels into planning models, and not least, the account taken for random (or dynamically adjusted) data by way of modeling expectation (stochastic approaches) or worst-case behavior (robust approaches).

Building on complementary expertise, our team’s overall goals are threefold:

(i) **Methodologies:** To design tight formulations for specific problems and generic models, relying on delayed cut and column generation, decomposition, extended formulations and projection tools for linear and nonlinear mixed integer programming models. More broadly, to contribute to theoretical and methodological developments of exact approaches in combinatorial optimization, while extending the scope of applications.
(ii) Problem solving: To demonstrate the strength of cooperation between complementary exact mathematical optimization techniques, dynamic programming, robust and stochastic optimization, constraint programming, combinatorial algorithms and graph theory, by developing “efficient” algorithms for specific mathematical models. To tackle large-scale real-life applications, providing provably good approximate solutions by combining exact methods and heuristics.

(iii) Software platform: To provide prototypes of specific model solvers and generic software tools that build on our research developments, writing code that serves as the proof-of-concept of the genericity and efficiency of our approaches, while transferring our research findings to internal and external users.

3. Research Program

3.1. Introduction

Combinatorial optimization is the field of discrete optimization problems. In many applications, the most important decisions (control variables) are binary (on/off decisions) or integer (indivisible quantities). Extra variables can represent continuous adjustments or amounts. This results in models known as mixed integer programs (MIP), where the relationships between variables and input parameters are expressed as linear constraints and the goal is defined as a linear objective function. MIPs are notoriously difficult to solve: good quality estimations of the optimal value (bounds) are required to prune enumeration-based global-optimization algorithms whose complexity is exponential. In the standard approach to solving an MIP is so-called branch-and-bound algorithm:

(i) one solves the linear programming (LP) relaxation using the simplex method;

(ii) if the LP solution is not integer, one adds a disjunctive constraint on a fractional component (rounding it up or down) that defines two sub-problems;

(iii) one applies this procedure recursively, thus defining a binary enumeration tree that can be pruned by comparing the local LP bound to the best known integer solution.

Commercial MIP solvers are essentially based on branch-and-bound (such IBM-CPLEX, FICO-Xpress-mp, or GUROBI). They have made tremendous progress over the last decade (with a speedup by a factor of 60). But extending their capabilities remains a continuous challenge; given the combinatorial explosion inherent to enumerative solution techniques, they remain quickly overwhelmed beyond a certain problem size or complexity.

Progress can be expected from the development of tighter formulations. Central to our field is the characterization of polyhedra defining or approximating the solution set and combinatorial algorithms to identify “efficiently” a minimum cost solution or separate an unfeasible point. With properly chosen formulations, exact optimization tools can be competitive with other methods (such as meta-heuristics) in constructing good approximate solutions within limited computational time, and of course has the important advantage of being able to provide a performance guarantee through the relaxation bounds. Decomposition techniques are implicitly leading to better problem formulation as well, while constraint propagation are tools from artificial intelligence to further improve formulation through intensive preprocessing. A new trend is robust optimization where recent progress have been made: the aim is to produce optimized solutions that remain of good quality even if the problem data has stochastic variations. In all cases, the study of specific models and challenging industrial applications is quite relevant because developments made into a specific context can become generic tools over time and see their way into commercial software.

Our project brings together researchers with expertise in mathematical programming (polyhedral approaches, decomposition and reformulation techniques in mixed integer programing, robust and stochastic programming, and dynamic programming), graph theory (characterization of graph properties, combinatorial algorithms) and constraint programming in the aim of producing better quality formulations and developing new methods to exploit these formulations. These new results are then applied to find high quality solutions for practical combinatorial problems such as routing, network design, planning, scheduling, cutting and packing problems, High Performance and Cloud Computing.
3.2. Polyhedral approaches for MIP

Adding valid inequalities to the polyhedral description of an MIP allows one to improve the resulting LP bound and hence to better prune the enumeration tree. In a cutting plane procedure, one attempt to identify valid inequalities that are violated by the LP solution of the current formulation and adds them to the formulation. This can be done at each node of the branch-and-bound tree giving rise to a so-called branch-and-cut algorithm [76]. The goal is to reduce the resolution of an integer program to that of a linear program by deriving a linear description of the convex hull of the feasible solutions. Polyhedral theory tells us that if \( X \) is a mixed integer program: \( X = P \cap \mathbb{Z}^n \times \mathbb{R}^p \) where \( P = \{ x \in \mathbb{R}^{n+p} : Ax \leq b \} \) with matrix \( (A, b) \in \mathbb{Q}^{m \times (n+p+1)} \), then \( \text{conv}(X) \) is a polyhedron that can be described in terms of linear constraints, i.e. it writes as \( \text{conv}(X) = \{ x \in \mathbb{R}^{n+p} : C x \leq d \} \) for some matrix \( (C, d) \in \mathbb{Q}^{m' \times (n+p+1)} \) although the dimension \( m' \) is typically quite large. A fundamental result in this field is the equivalence of complexity between solving the combinatorial optimization problem \( \min \{ cx : x \in X \} \) and solving the separation problem over the associated polyhedron \( \text{conv}(X) \): if \( \bar{x} \notin \text{conv}(X) \), find a linear inequality \( \pi x \geq \pi_0 \) satisfied by all points in \( \text{conv}(X) \) but violated by \( \bar{x} \). Hence, for NP-hard problems, one can not hope to get a compact description of \( \text{conv}(X) \) nor a polynomial time exact separation routine. Polyhedral studies focus on identifying some of the inequalities that are involved in the polyhedral description of \( \text{conv}(X) \) and derive efficient separation procedures (cutting plane generation). Only a subset of the inequalities \( C x \leq d \) can offer a good approximation, that combined with a branch-and-bound enumeration techniques permits to solve the problem. Using cutting plane algorithm at each node of the branch-and-bound tree, gives rise to the algorithm called branch-and-cut.

3.3. Decomposition and reformulation approaches

An hierarchical approach to tackle complex combinatorial problems consists in considering separately different substructures (subproblems). If one is able to implement relatively efficient optimization on the substructures, this can be exploited to reformulate the global problem as a selection of specific subproblem solutions that together form a global solution. If the subproblems correspond to subset of constraints in the MIP formulation, this leads to Dantzig-Wolfe decomposition [7], [9], [8]. If it corresponds to isolating a subset of decision variables, this leads to Bender’s decomposition. Both lead to extended formulations of the problem with either a huge number of variables or constraints. Dantzig-Wolfe approach requires specific algorithmic approaches to generate subproblem solutions and associated global decision variables dynamically in the course of the optimization. This procedure is known as column generation, while its combination with branch-and-bound enumeration is called branch-and-price. Alternatively, in Bender’s approach, when dealing with exponentially many constraints in the reformulation, the cutting plane procedures that we defined in the previous section are well-suited tools. When optimization on a substructure is (relatively) easy, there often exists a tight reformulation of this substructure typically in an extended variable space. This gives rise powerful reformulation of the global problem, although it might be impractical given its size (typically pseudo-polynomial). It can be possible to project (part of) the extended formulation in a smaller dimensional space if not the original variable space to bring polyhedral insight (cuts derived through polyhedral studies can often be recovered through such projections).

3.4. Integration of Artificial Intelligence Techniques in Integer Programming

When one deals with combinatorial problems with a large number of integer variables, or tightly constrained problems, mixed integer programming (MIP) alone may not be able to find solutions in a reasonable amount of time. In this case, techniques from artificial intelligence can be used to improve these methods. In particular, we use variable fixing techniques, primal heuristics and constraint programming.

Primal heuristics are useful to find feasible solutions in a small amount of time. We focus on heuristics that are either based on integer programming (rounding, diving, relaxation induced neighborhood search, feasibility pump), or that are used inside our exact methods (heuristics for separation or pricing subproblem, heuristic constraint propagation, ...). Such methods are likely to produce good quality solutions only if the integer programming formulation is of top quality, i.e., if its LP relaxation provides a good approximation of the IP solution.
In the same line, variable fixing techniques, that are essential in reducing the size of large scale problems, rely on good quality approximations: either tight formulations or tight relaxation solvers (as a dynamic program combined with state space relaxation). Then if the dual bound derives when the variable is fixed to one exceeds the incumbent solution value, the variable can be fixed to zero and hence removed from the problem. The process can be apply sequentially by refining the degree of relaxation.

Constraint Programming (CP) focuses on iteratively reducing the variable domains (sets of feasible values) by applying logical and problem-specific operators. The latter propagates on selected variables the restrictions that are implied by the other variable domains through the relations between variables that are defined by the constraints of the problem. Combined with enumeration, it gives rise to exact optimization algorithms. A CP approach is particularly effective for tightly constrained problems, feasibility problems and min-max problems. Mixed Integer Programming (MIP), on the other hand, is known to be effective for loosely constrained problems and for problems with an objective function defined as the weighted sum of variables. Many problems belong to the intersection of these two classes. For such problems, it is reasonable to use algorithms that exploit complementary strengths of Constraint Programming and Mixed Integer Programming.

3.5. Robust Optimization

Decision makers are usually facing several sources of uncertainty, such as the variability in time or estimation errors. A simplistic way to handle these uncertainties is to overestimate the unknown parameters. However, this results in over-conservatism and a significant waste in resource consumption. A better approach is to account for the uncertainty directly into the decision aid model by considering mixed integer programs that involve uncertain parameters. Stochastic optimization account for the expected realization of random data and optimize an expected value representing the average situation. Robust optimization on the other hand entails protecting against the worst-case behaviour of unknown data. There is an analogy to game theory where one considers an oblivious adversary choosing the realization that harms the solution the most. A full worst case protection against uncertainty is too conservative and induces very high over-cost. Instead, the realization of random data are bound to belong to a restricted feasibility set, the so-called uncertainty set. Stochastic and robust optimization rely on very large scale programs where probabilistic scenarios are enumerated. There is hope of a tractable solution for realistic size problems, provided one develops very efficient ad-hoc algorithms. The techniques for dynamically handling variables and constraints (column-and-row generation and Bender’s projection tools) that are at the core of our team methodological work are specially well-suited to this context.

3.6. Polyhedral Combinatorics and Graph Theory

Many fundamental combinatorial optimization problems can be modeled as the search for a specific structure in a graph. For example, ensuring connectivity in a network amounts to building a tree that spans all the nodes. Inquiring about its resistance to failure amounts to searching for a minimum cardinality cut that partitions the graph. Selecting disjoint pairs of objects is represented by a so-called matching. Disjunctive choices can be modeled by edges in a so-called conflict graph where one searches for stable sets — a set of nodes that are not incident to one another. Polyhedral combinatorics is the study of combinatorial algorithms involving polyhedral considerations. Not only it leads to efficient algorithms, but also, conversely, efficient algorithms often imply polyhedral characterizations and related min-max relations. Developments of polyhedral properties of a fundamental problem will typically provide us with more interesting inequalities well suited for a branch-and-cut algorithm to more general problems. Furthermore, one can use the fundamental problems as new building bricks to decompose the more general problem at hand. For problem that let themselves easily be formulated in a graph setting, the graph theory and in particular graph decomposition theorem might help.

4. Application Domains

4.1. Introduction
Our group has tackled applications in logistics, transportation and routing [33] [14] [75], [74], [70], [72], in production planning [92] and inventory control [70], [72], in network design and traffic routing [53], [62], [68], [95], [50], [63], [80], [88], in cutting and placement problems [77], [78], [89], [90], [91], [93], and in scheduling [86], [81], [46], and in High Performance and Cloud Computing [20] [40] [41] [34] [48] [47].

4.2. Network Design and Routing Problems

We are actively working on problems arising in network topology design, implementing a survivability condition of the form “at least two paths link each pair of terminals”. We have extended polyhedral approaches to problem variants with bounded length requirements and re-routing restrictions [62]. Associated to network design is the question of traffic routing in the network: one needs to check that the network capacity suffices to carry the demand for traffic. The assignment of traffic also implies the installation of specific hardware at transient or terminal nodes.

To accommodate the increase of traffic in telecommunication networks, today’s optical networks use grooming and wavelength division multiplexing technologies. Packing multiple requests together in the same optical stream requires to convert the signal in the electrical domain at each aggregation of disaggregation of traffic at an origin, a destination or a bifurcation node. Traffic grooming and routing decisions along with wavelength assignments must be optimized to reduce opto-electronic system installation cost. We developed and compared several decomposition approaches [97], [96], [95] to deal with backbone optical network with relatively few nodes (around 20) but thousands of requests for which traditional multi-commodity network flow approaches are completely overwhelmed. We also studied the impact of imposing a restriction on the number of optical hops in any request route [94]. We also developed a branch-and-cut approach to a problem that consists in placing sensors on the links of a network for a minimum cost [68], [69].

![Design of a SDH/SONET european network where demands are multiplexed.](image)

We studied several time dependent formulations for the unit demand vehicle routing problem [55], [54]. We gave new bounding flow inequalities for a single commodity flow formulation of the problem. We described their impact by projecting them on some other sets of variables, such as variables issued of the Picard and
Queyranne formulation or the natural set of design variables. Some inequalities obtained by projection are facet defining for the polytope associated with the problem. We are now running more numerical experiments in order to validate in practice the efficiency of our theoretical results.

We also worked on the p-median problem, applying the matching theory to develop an efficient algorithm in Y-free graphs and to provide a simple polyhedral characterization of the problem and therefore a simple linear formulation [87] simplifying results from Baiou and Barahona.

We considered the multi-commodity transportation problem. Applications of this problem arise in, for example, rail freight service design, "less than truckload" trucking, where goods should be delivered between different locations in a transportation network using various kinds of vehicles of large capacity. A particularity here is that, to be profitable, transportation of goods should be consolidated. This means that goods are not delivered directly from the origin to the destination, but transferred from one vehicle to another in intermediate locations. We proposed an original Mixed Integer Programming formulation for this problem which is suitable for resolution by a Branch-and-Price algorithm and intelligent primal heuristics based on it.

For the problem of routing freight railcars, we proposed two algorithms based on the column generation approach. These algorithms have been tested on a set of real-life instances coming from a real Russian freight transportation company. Our algorithms have been faster on these instances than the current solution approach being used by the company.

4.3. Packing and Covering Problems

Realopt team has a strong experience on exact methods for cutting and packing problems. These problems occur in logistics (loading trucks), industry (wood or steel cutting), computer science (parallel processor scheduling).

We developed a branch-and-price algorithm for the Bin Packing Problem with Conflicts which improves on other approaches available in the literature [85]. The algorithm uses our methodological advances like the generic branching rule for the branch-and-price and the column based heuristic. One of the ingredients which contributes to the success of our method are fast algorithms we developed for solving the subproblem which is the Knapsack Problem with Conflicts. Two variants of the subproblem have been considered: with interval and arbitrary conflict graphs.

We also developed a branch-and-price algorithm for a variant of the bin-packing problem where the items are fragile. In [44] we studied empirically different branching schemes and different algorithms for solving the subproblems.

We studied a variant of the knapsack problem encountered in inventory routing problem [72]: we faced a multiple-class integer knapsack problem with setups [71] (items are partitioned into classes whose use implies a setup cost and associated capacity consumption). We showed the extent to which classical results for the knapsack problem can be generalized to this variant with setups and we developed a specialized branch-and-bound algorithm.

We studied the orthogonal knapsack problem, with the help of graph theory [65], [64], [67], [66]. Fekete and Schepers proposed to model multi-dimensional orthogonal placement problems by using an efficient representation of all geometrically symmetric solutions by a so called packing class involving one interval graph for each dimension. Though Fekete & Schepers’ framework is very efficient, we have however identified several weaknesses in their algorithms: the most obvious one is that they do not take advantage of the different possibilities to represent interval graphs. We propose to represent these graphs by matrices with consecutive ones on each row. We proposed a branch-and-bound algorithm for the 2D knapsack problem that uses our 2D packing feasibility check. We are currently developing exact optimization tools for glass-cutting problems in a collaboration with Saint-Gobain [35]. This 2D-3stage-Guillotine cut problems are very hard to solve given the scale of the instance we have to deal with. Moreover one has to issue cutting patterns that avoid the defaults that are present in the glass sheet that are used as raw material. There are extra sequencing constraints regarding the production that make the problem even more complex.
We have also organized a European challenge on packing with society Renault: see http://challenge-esicup-2015.org/. This challenge is about loading trucks under practical constraints.

4.4. Planning, Scheduling, and Logistic Problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. We considered an industrial application where one must construct the planning of single product pickups over time; each site accumulates stock at a deterministic rate; the stock is emptied on each visit. We have developed a branch-and-price algorithm where periodic plans are generated for vehicles by solving a multiple choice knapsack subproblem, and the global planning of customer visits is coordinated by the master program [73]. We previously developed approximate solutions to a related problem combining vehicle routing and planning over a fixed time horizon (solving instances involving up to 6000 pick-ups and deliveries to plan over a twenty day time horizon with specific requirements on the frequency of visits to customers [75].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [79] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximize the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [61] and exact algorithms [46]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [45]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [81]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [83]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [84], [82].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [43], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [42] contains a detailed investigation of what makes solving the MIP formulations of such problems challenging; it provides a survey of the known methods for strengthening formulations for these applications, and it also pinpoints the specific substructure that seems to cause the bottleneck in solving these models. Finally, the results of [49] provide demonstrably stronger formulations for some problem classes than any previously proposed. We are now working on planning phytosanitary treatments in vineries.

We have been developing robust optimization models and methods to deal with a number of applications like the above in which uncertainty is involved. In [57], [56], we analyzed fundamental MIP models that incorporate uncertainty and we have exploited the structure of the stochastic formulation of the problems in order to derive algorithms and strong formulations for these and related problems. These results appear to be the first of their kind for structured stochastic MIP models. In addition, we have engaged in successful research to apply concepts such as these to health care logistics [51]. We considered train timetabling problems and their re-optimization after a perturbation in the network [59], [58]. The question of formulation is central. Models of the literature are not satisfactory: continuous time formulations have poor quality due to the presence of discrete decision (re-sequencing or re-routing); arc flow in time-space graph blow-up in size (they can only handle a single line timetabling problem). We have developed a discrete time formulation that strikes a compromise between these two previous models. Based on various time and network aggregation strategies, we develop a 2-stage approach, solving the contiguous time model having fixed the precedence based on a solution to the discrete time model.

Currently, we are conducting investigations on a real-world planning problem in the domain of energy production, in the context of a collaboration with EDF [26], [27], [28]. The problem consists in scheduling maintenance periods of nuclear power plants as well as production levels of both nuclear and conventional power plants in order to meet a power demand, so as to minimize the total production cost. For this application,
we used a Dantzig-Wolfe reformulation which allows us to solve realistic instances of the deterministic version of the problem [60]. In practice, the input data comprises a number of uncertain parameters. We deal with a scenario-based stochastic demand with help of a Benders decomposition method. We are working on Multistage Robust Optimization approaches to take into account other uncertain parameters like the duration of each maintenance period, in a dynamic optimization framework. The main challenge addressed in this work is the joint management of different reformulations and solving techniques coming from the deterministic (Dantzig-Wolfe decomposition, due to the large scale nature of the problem), stochastic (Benders decomposition, due to the number of demand scenarios) and robust (reformulations based on duality and/or column and/or row generation due to maintenance extension scenarios) components of the problem [52].

4.5. Resource Allocation for High Performance and Cloud Computing

In the context of numerical simulations on high performance machines, optimizing data locality and resource usage is very important for faster execution times and lower energy consumption. This optimization can be seen as a special case of scheduling problem on parallel resource, with several challenges. First, instances are typically large: a large matrix factorization (with $50 \times 50$ blocks) involves about $30 \cdot 10^3$ tasks. Then, HPC platforms consist of heterogeneous and unrelated resources, what is known to make scheduling problems hard to approximate. Finally, due to co-scheduling effects and shared communication resources, it is not realistic to accurately model the exact duration of tasks. All these observations make it impossible to rely on static optimal solutions, and HPC applications have gone from simple generic static allocations to runtime dynamic scheduling strategies that make their decisions based on the current state of the platform (the location of input data), the expected transfer and running times for the tasks, and some affinity and priority information that have possibly been computed offline. In this context, we are strongly involved in the design of scheduling strategies for the StarPU runtime, with two goals: proving that it is possible to design approximation algorithms whose complexity is extremely small (typically sub-linear in the number of ready tasks), and show that they can be used in practice with good performance results. We are pursuing collaborations both with teams developing the StarPU system (Storm) by designing algorithms for the generic scheduling problems [20], and with teams developing linear algebra algorithms over the runtime (Hiepacs), by proposing specialized algorithms for specific cases. For example, in the case of linear algebra applications on heterogeneous platforms, we have considered the combinatorial optimization problem associated to matrix multiplication, that is amenable to partitioning the unit square into zones of prescribed areas while minimizing the overall size of the boundaries. We have improved the best known approximation ratio to 1.15 in [40] and we have shown that the resulting distribution schemes can indeed be used to design efficient implementations using StarPU in [41].

In the context of Cloud Computing platforms and Data Science, we are interested in resource allocation and data placement strategies. For BigData applications running on data centers platforms, data locality is the largest contributing factor to application performance. In practice, allocation decisions are made at runtime based on strategies that tend to favor local tasks. Our goal is to assess and to improve the efficiency of these runtime strategies. In particular, we have proven that the problem of maximizing locality when allocating map tasks is amenable to a graph orientation and a semi matching problem, what enabled us to assess the efficiency of classical MapReduce allocation algorithm in [34] for the map phase and to propose a low cost algorithm to compute optimal allocation schemes. We also consider more generic VM placement problem for large-scale datacenters. This placement is often handled with naive greedy rules, whereas it is possible to propose online or offline efficient allocation algorithms, for example to optimize the reliability of all applications in a platform with faults [48] or to co-locate applications with compatible periodic load variations [47].

5. Highlights of the Year

5.1. Highlights of the Year

Olivier Beaumont was the Track Chair of the Algorithm Track of Super Computing 2017 (November, Denver, USA); “The International Conference for High Performance Computing, Networking, Storage and Analysis” https://sc17.supercomputing.org. SuperComputing is the major international conference on High Performance Computing.
We have contributed to the JULIA mathematical programming ecosystem by providing tools to decompose a mixed integer programming model into blocks. This makes it very convenient to model Benders or Dantzig-Wolfe decomposition using JUMP and to compare different decomposition for a given problem formulation.

Our generic software platform BaPCod is now giving rise to specific branches for classes of applications. The first such release concerns the classic benchmark Vehicle Routing Problem variants that arise in logistics. The methods that are build in the platform emerge from our collaboration with our Brazilian partners of the SAMBA associated team. For their anterior work, our partners have received the 2017 best paper award from the prestigious journal “Mathematical Programming Computation”. With the new version that is built under BaPCod, we have managed to solve to optimality many more open instances of classic and very competitive Vehicle Routing Problem with Time Windows [37]. This study has been an opportunity to improve significantly the performance on the generic Branch-Cut-and-Price platform and to highlight the interests of such generic methodologies.

6. New Software and Platforms

6.1. BaPCod

A generic Branch-And-Price-And-Cut Code


**FUNCTIONAL DESCRIPTION**: BaPCod is a prototype code that solves Mixed Integer Programs (MIP) by application of reformulation and decomposition techniques. The reformulated problem is solved using a branch-and-price-and-cut (column generation) algorithms, Benders approaches, network flow and dynamic programming algorithms. These methods can be combined in several hybrid algorithms to produce exact or approximate solutions (primal solutions with a bound on the deviation to the optimum).

- Participants: Artur Alves Pessoa, Boris Detienne, Eduardo Uchoa Barboza, Franck Labat, François Clautiaux, François Vanderbeck, Halil Sen, Issam Tahiri, Michael Poss, Pierre Pesneau, Romain Leguay and Ruslan Sadykov
- Partners: Université de Bordeaux - CNRS - IPB - Universidade Federal Fluminense
- Contact: François Vanderbeck
- URL: https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod

6.2. WineryPlanning

- Participants: Agnes Le Roux, Alexis Toullat, François Vanderbeck, Issam Tahiri and Ruslan Sadykov
- Contact: François Vanderbeck

6.3. ORTOJ

*Operation Research Tools Under Julia*

**KEYWORDS**: Modeling - Processing - Dashboard

**FUNCTIONAL DESCRIPTION**: This set of tools currently includes : 1) BlockJuMP.jl: extension of JuMP to model decomposable mathematical programs (using either Benders or Dantzig-Wolfe decomposition paradigm) 2) Scanner.jl: a default data parser to ease the reading of the input data in the form that they are often encountered in operational research. 3) BenchmarkUtils.jl: Tools to ease the setup of numerical experiments to benchmark algorithmic feature performances. The test automation permits to quickly calibrate the parameters of an arbitrary algorithm control function.

- Participants: François Vanderbeck, Guillaume Marques, Issam Tahiri and Ruslan Sadykov
- Contact: Issam Tahiri
7. New Results

7.1. Improving Branch-and-Price Methods

We have made progress on stabilization techniques and math-heuristics that are essential components for generic Branch-and-Price methods.

The convergence of a column generation algorithm can be improved in practice by using stabilization techniques. Smoothing and proximal methods based on penalizing the deviation from the incumbent dual solution have become standards of the domain. Interpreting column generation as cutting plane strategies in the dual problem, we have analyzed [15] the mechanisms on which stabilization relies. In particular, the link is established between smoothing and in-out separation strategies to derive generic convergence properties. For penalty function methods as well as for smoothing, we describe proposals for parameter self-adjusting schemes. Such schemes make initial parameter tuning less of an issue as corrections are made dynamically. Such adjustments also allow to adapt the parameters to the phase of the algorithm. Extensive test reports validate our self-adjusting parameter scheme and highlight their performances. Our results also show that using smoothing in combination with penalty function yields a cumulative effect on convergence speed-ups.

Math heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending MIP based heuristics, we have studied [17] generic procedures to build primal solutions in the context of a branch-and-price approach. As the Dantzig-Wolfe reformulation of a problem is typically tighter than that of the original compact formulation, heuristics based on rounding its linear programing (LP) solution can be more competitive. We focus on the so-called diving methods that used re-optimization after each LP rounding. We explore combination with diversification- intensification paradigms such as Limited Discrepancy Search, sub-MIPing, relaxation induced neighbourhood search, local branching, and strong branching. The dynamic generation of variables inherent to a column generation approach requires specific adaptation of heuristic paradigms. We manage to use simple strategies to get around these technical issues. Our numerical results on generalized assignment, cutting stock, and vertex coloring problems sets new benchmarks, highlighting the performance of diving heuristics as generic procedures in a column generation context and producing better solutions than state-of-the-art specialized heuristics in some cases.

7.2. Aggregation Techniques

We have developed [13] a general solution framework based on aggregation techniques to solve NP-Hard problems that can be formulated as a circulation model with specific side constraints. The size of the extended Mixed Integer Linear Programming formulation is generally pseudo-polynomial. To efficiently solve exactly these large scale models, we propose a new iterative aggregation and disaggregation algorithm. At each iteration, it projects the original model onto an aggregated one, producing an approximate model. The process iterates to refine the current aggregated model until the optimality is proved.

The computational experiments on two hard optimization problems (a variant of the vehicle routing problem and the cutting-stock problem) show that a generic implementation of the proposed framework allows us to outperform previous known methods.

We have applied this aggregation method to reduce the size of column generation (CG) models for covering problems in which the feasible subsets depend on a resource constraint [16]. The aggregation relies on a correlation between the resource consumption of the elements and the corresponding optimal dual values. The resulting aggregated dual model is a restriction of the original one, and it can be rapidly optimized to obtain a feasible dual solution. A primal bound can also be obtained by restricting the set of columns to those saturated by the dual feasible solution obtained by aggregation. The convergence is realized by iterative disaggregation until the gap is closed by the bounds. Computational results show the usefulness of our method for different cutting-stock problems. An important advantage is the fact that it can produce high-quality dual bounds much faster than the traditional Lagrangian bound used in stabilized column generation.
We have developed an algorithm for the exact solution of the Temporal Knapsack Problem [29], [24]. We proposed a dynamic programming formulation for the problem, whose size is exponential in the size of the input data. To cope with the curse of dimensionality, we based our algorithm on the Successive Sublimation Dynamic Programming method. We generalized it to allow more precise aggregation of the state space of the dynamic program. Several application-specific feasibility tests and dominance relations, based on aggregated information, are used to derive an efficient implementation of the method. The algorithms compares favorably with the literature, solving several open instances.

7.3. Revisiting Benders Decomposition & Enhancing the Algorithm

In Benders decomposition approach to mixed integer programs, the optimization is carried in two stages: key first-stage decision variables are optimized using a polyhedral approximation of the full-blown problem projection, then a separation problem expressed in the second-stage variables is solved to check if the current first-stage solution is truly feasible, and otherwise, it produces a violated inequality. Such cutting-plane algorithms suffer from several drawbacks and may have very bad convergence rates. We have reviewed [98] the battery of approaches that have been proposed in the literature to address these drawbacks and to speed-up the algorithm. Our contribution consists in explaining these techniques in simple terms and unified notations, showing that in several cases, different proposals of the literature boil down to the same key ideas. We classify methods into specific initialization mode, stabilization techniques, strategies to select the separation point, and cut generation strategies. We have contributed to enhance convergence of Benders cutting plane algorithm by a mixture of smoothing techniques and proximal approaches. Our numerical benchmarking is still on going [18].

7.4. Routing Problems

Given a directed graph $G = (V, A)$, a cost function $c$ associated with the arcs of $A$, and a set of precedence constraints $B \subseteq V \times V$, the Precedence Constrained Asymmetric Traveling Salesman Problem (PCATSP) seeks for a minimum cost Hamiltonian circuit, starting at node 1, and such that for each $(i, j) \in B$, the node $i$ is visited before node $j$. There are many ways of modelling the ATSP and several for the PCATSP. In [14], [25] we present new formulations for the two problems that can be viewed as resulting from combining precedence variable based formulations with network flow based formulations. Indeed, the former class of formulations permits to integrate linear ordering constraints. The motivating formulation for this work is a complicated and “ugly” formulation that results from the separation of generalized subtour elimination constraints presented. This so called “ugly” formulation exhibits, however, one interesting feature, namely the “disjoint subpaths” property that is further explored to create more complicated formulations that combine two (or three) “disjoint path” network flow based formulations and have a stronger linear programming bound. Some of these stronger formulations are related to the ones presented for the PCATSP and can be viewed as generalizations in the space of the precedence based variables. Several sets of projected inequalities in the space of the arc and precedence variables are obtained by projection from these network flow based formulations. Computational results for the ATSP and PCATSP evaluate the quality of the new models and inequalities.

In [36] we deal with the Minimum Latency Problem (MLP), another variant of the well-known Traveling Salesman Problem in which the objective is to minimize the sum of waiting times of customers. This problem arises in many applications where customer satisfaction is more important than the total time spent by the server. This paper presents a novel branch-and-price algorithm for MLP that strongly relies on new features for the ng-path relaxation, namely: (1) a new labeling algorithm with an enhanced dominance rule named multiple partial label dominance; (2) a generalized definition of ng-sets in terms of arcs, instead of nodes; and (3) a strategy for decreasing ng-set sizes when those sets are being dynamically chosen. Also, other elements of efficient exact algorithms for vehicle routing problems are incorporated into our method, such as reduced cost fixing, dual stabilization, route enumeration and strong branching. Computational experiments over TSPLIB instances are reported, showing that several instances not solved by the current state-of-the-art method can now be solved.
In [37], [31] we consider the Resource Constrained Shortest Path problem arising as a subproblem in state-of-the-art Branch-Cut-and-Price algorithms for vehicle routing problems. We propose a variant of the bidirectional label correcting algorithm in which the labels are stored and extended according to so-called bucket graph. Such organization of labels helps to decrease significantly the number of dominance checks and the running time of the algorithm. We also show how the forward/backward route symmetry can be exploited and how to filter the bucket graph using reduced costs. The proposed algorithm can be especially beneficial for vehicle routing instances with large vehicle capacity and/or with time constraints. Computational experiments were performed on instances from the distance constrained vehicle routing problem, including multi-depot and site-depended variants, on the vehicle routing problem with time windows, and on the “nightmare” instances of the heterogeneous fleet vehicle routing problem. Very significant improvements over the best algorithms in the literature were achieved and many instances could be solved for the first time.

We also considered a family of Vehicle Routing Problem (VRP) variants that generalize the classical Capacitated VRP by taking into account the possibility that vehicles differ by capacity, costs, depot allocation, or even by the subset of customers that they can visit. In [33], [30], [23] we propose a branch-cut-and-price algorithm that adapts advanced features found in the best performing exact algorithms for homogeneous fleet VRPs. The original contributions include: (i) the use of Extended Capacity Cuts, defined over a pseudo-polynomially large extended formulation, together with Rank-1 Cuts, defined over the Set Partitioning Formulation; (ii) the concept of vehicle-type dependent memory for Rank-1 Cuts; and (iii) a new family of lifted Extended Capacity Cuts that takes advantage of the vehicle-type dependent route enumeration. The algorithm was extensively tested in instances of the literature and was shown to be significantly better than previous exact algorithms, finding optimal solutions for many instances with up to 200 customers and also for some larger instances. Several new best solutions were found too.

7.5. Machine Scheduling Problems

In [21] we consider the unrelated parallel machine scheduling problem with setup times to minimize a general objective function. In this work we present a novel exact algorithm that is capable of solving this problem \( R[r_j, s^h_j, \sum f_j(C_j) \] and the large class of problems that can be derived as particular cases from it. The proposed algorithm consists of a branch-cut-and-price approach that combines several features such as non-robust cuts, strong branching, reduced cost fixing and dual stabilization. To our knowledge, this is the first exact algorithm for unrelated machines with earliness and/or tardiness criteria that can solve consistently instances with more than 20 jobs. We report improved bounds for instances of problems \( R[r_j, s^h_j, \sum w'_j E_j + w_j T_j \] and \( R[\sum w'_j E_j + w_j T_j \] with up to 80 and 120 jobs, respectively.

7.6. Scheduling Strategies for Runtime Systems

We consider the design of low cost but guaranteed approximation algorithms in the context of the runtime StarPU in [20]. In High Performance Computing, heterogeneity is now the norm with specialized accelerators like GPUs providing efficient computational power. The added complexity has led to the development of task-based runtime systems, which allow complex computations to be expressed as task graphs, and rely on scheduling algorithms to perform load balancing between all resources of the platforms. Developing good scheduling algorithms, even on a single node, and analyzing them can thus have a very high impact on the performance of current HPC systems. The special case of two types of resources (namely CPUs and GPUs) is of practical interest. HeteroPrio is such an algorithm which has been proposed in the context of fast multipole computations, and then extended to general task graphs with very interesting results. In this paper, we provide a theoretical insight on the performance of HeteroPrio, by proving approximation bounds compared to the optimal schedule in the case where all tasks are independent and for different platform sizes. Interestingly, this shows that spoliation allows to prove approximation ratios for a list scheduling algorithm on two unrelated resources, which is not possible otherwise. We also establish that almost all our bounds are tight. Additionally, we provide an experimental evaluation of HeteroPrio on real task graphs from dense linear algebra computation, which highlights the reasons explaining its good practical performance.
7.7. Matrix Partitioning for Parallel Computing on Heterogeneous Platforms

We consider the combinatorial optimization problem that arises in the context of matrix multiplication in [40]. The problem of partitioning a matrix into a set of sub-matrices has received increased attention recently and is crucial when considering dense linear algebra and kernels with similar communication patterns on heterogeneous platforms. The problem of load balancing and minimizing communication is traditionally reducible to an optimization problem that involves partitioning a square into rectangles. This problem has been proven to be NP-Complete for an arbitrary number of partitions. In this paper, we present recent approaches that relax the restriction that all partitions be rectangles. The first approach uses an original mathematical technique to find the exact optimal partitioning. Due to the complexity of the technique, it has been developed for a small number of partitions only. However, even at a small scale, the optimal partitions found by this approach are often non-rectangular and sometimes non-intuitive. The second approach is the study of approximate partitioning methods by recursive partitioning algorithms. In particular we use the work on optimal partitioning to improve pre-existing algorithms. In this paper we discuss the different perspectives it opens and present two algorithms, SNRPP which is a $\sqrt{\frac{3}{2}}$ approximation, and NRPP which is a $\frac{2}{\sqrt{3}}$ approximation. While sub-optimal, this approach works for an arbitrary number of partitions. We use the first exact approach to analyse how close to the known optimal solutions the NRPP algorithm is for small numbers of partitions. In order to validate above approach, we consider in [41] how to allocate data when performing matrix multiplication on a heterogeneous node, with multicores and GPUs. Classical (cyclic) allocations designed for homogeneous settings are not appropriate, but the advent of task-based runtime systems makes it possible to use more general allocations. Previous theoretical work has proposed square and cube partitioning algorithms aimed at minimizing data movement for matrix multiplication. We propose techniques to adapt these continuous square partitionings to allocating discrete tiles of a matrix, and strategies to adapt the static allocation at run-time. We use these techniques in an implementation of Matrix Multiplication based on the StarPU runtime system, and we show through extensive experiments that this implementation allows to consistently obtain a lower communication volume while improving slightly the execution time, compared to standard state-of-the-art dynamic strategies.

7.8. Convergence between HPC and Data Science

We consider the use of replication when scheduling independent identical tasks in [34]. MapReduce is a well-know framework for distributing data-processing computations onto parallel clusters. In MapReduce, a large computation is broken into small tasks that run in parallel on multiple machines, and scales easily to very large clusters of inexpensive commodity computers. Before the Map phase, the original dataset is split into data chunks that are replicated (a constant number of times, usually 3) and distributed randomly onto computing nodes. During the Map phase, local tasks (i.e., tasks whose data chunks are stored locally) are assigned in priority when processors request tasks. In this paper, we provide the first complete theoretical analysis of data locality in the Map phase of MapReduce, and more generally, for bag-of-tasks applications that behave like MapReduce. We prove that if tasks are homogeneous (in terms of processing time), as soon as the replication factor is larger than 2, FindAssignment, a matching based algorithm, achieves a quasi-perfect makespan (i.e., optimal up to an additive constant of one step) using a sophisticated matching algorithm. Above result is proved with high probability when the number of tasks becomes arbitrarily large, and we therefore complement theoretical results with simulations that corroborate them even for small number of tasks. We also show that the matching-based approach leads to an improvement of data locality during the Map phase and therefore decreases the amount of communications needed to achieve perfect makespan, compared to the classical MapReduce greedy approach. In the context of the convergence between HPC and Data Science, we investigate the use of Burst Buffers for HPC applications in [38]. Burst-Buffers are high throughput, small size intermediate storage systems typically based on SSDs or NVRAM that are designed to be used as a potential buffer between the computing nodes of a supercomputer and its main storage system consisting of hard drives. Their purpose is to absorb the bursts of I/O that many HPC applications experience (for example for saving checkpoints or data from intermediate results). In this paper, we propose a probabilistic model for evaluating the performance of Burst-Buffers. From a model of application and a data management strategy, we build a Markov chain based model of the system, that allows to quickly answer issues about dimensioning of the
system: for a given set of applications, and for a given Burst-Buffer size and bandwidth, how often does the buffer overflow? We also provide extensive simulation results to validate our modeling approach.

7.9. Network Design Problems

The delivery of freight from manufacturing platforms to demand zones is often managed through one or more intermediate locations where storing, merging, transshipment and consolidation activities are performed. In [22], we design a Two-Echelon Distribution Network that helps synchronize different flows of product. Under demand uncertainty, our model integrates decisions on the locations and the size of second echelon facilities and decisions on the flow assignment between the echelons, and on delivery routes to serve the demand zones.

7.10. Two-dimensional Guillotine Cutting Problems

The two-dimensional knapsack problem consists in packing a set of small rectangular items into a given large rectangle while maximizing the total reward associated with selected items. In [13], we restrict our attention to packings that emanate from a k-stage guillotine-cut process. We introduce a generic model where a knapsack solution is represented by a flow in a directed acyclic hypergraph. This hypergraph model derives from a forward labeling dynamic programming recursion that enumerates all non-dominated feasible cutting patterns. To reduce the hypergraph size, we make use of further dominance rules and a filtering procedure based on Lagrangian reduced costs fixing of hyperarcs. Our hypergraph model is (incrementally) extended to account for explicit bounds on the number of copies of each item. Our exact forward labeling algorithm is numerically compared to solving the max-cost flow model in the base hypergraph with side constraints to model production bounds. Benchmarks are reported on instances from the literature and on datasets derived from a real-world application.

Also we consider a variant of two-dimensional guillotine cutting-stock problem that arises when different bills of order (or batches) are considered consecutively. The raw material leftover of the last cutting pattern is not counted as waste as it can be reused for cutting the next batch. The objective is thus to maximize the length of the leftover. In [35], [32] we propose a diving heuristic based on a Dantzig-Wolfe reformulation solved by column generation in which the pricing problem is solved using dynamic programming (DP). This DP generates so-called non-proper columns, i.e. cutting patterns that cannot participate in a feasible integer solution of the problem. We show how to adapt the standard diving heuristic to this “non-proper” case while keeping its effectiveness. We also introduce the partial enumeration technique, which is designed to reduce the number of non-proper patterns in the solution space of the dynamic program. This technique helps to strengthen the lower bounds obtained by column generation and improve the quality of solutions found by the diving heuristic. Computational results are reported and compared on classical benchmarks from the literature as well as on new instances inspired from industrial data. According to these results, proposed diving algorithms outperform constructive and evolutionary heuristics.

7.11. On sets avoiding distance 1

In a joint work with C. Bachoc, T. Bellitto and P. Moustrou [39], we consider the maximum density of sets avoiding distance 1 in \( \mathbb{R}^n \). Let \( ||.|| \) be a norm of \( \mathbb{R}^n \) and \( G(||.||) \) be the so-called unit distance graph with the points of \( \mathbb{R}^n \) as vertex set and for edge set, the set of pairs \( \{x, y\} \) such that \( ||x - y|| = 1 \). An independent set of \( G(||.||) \) is said to avoid distance 1.

Let \( ||.||_E \) denote the Euclidean norm. For \( n = 2 \), the chromatic number of \( G(||.||_E) \) is still wide open: it is only known that \( 4 \leq \chi (G(||.||_E)) \leq 7 \) (Nelson, Isbell 1950). The measurable chromatic number \( \chi_m \) of the graph \( G(||.||) \) is the minimal number of measurable stable sets of \( G(||.||) \) needed to cover all its vertices. Obviously, we have \( \chi (G(||.||_E)) \leq \chi_m (G(||.||_E)) \). For \( n = 2 \), \( 5 \leq \chi_m (G(||.||_E)) \) (Falconer 1981).
Let $m_1(G_{||.||})$ denote the maximum density of a measurable set avoiding distance 1. We have $m_1(G_{||.||}) \leq \chi m(G_{||.||})$. We study the maximum density $m_1$ for norms defined by polytopes: if $P$ is a centrally symmetric polytope and $x$ is a point of $R^n$, $||x||_P$ is the smallest positive real $t$ such that $x \in tP$. Polytope norms include some usual norms such as the $L^1$ and $L^\infty$ norms.

If $P$ tiles the space by translation, then it is easy to see that $m_1(G_{||.||}_P) \geq \frac{1}{2^n}$. C. Bachoc and S. Robins conjectured that equality always holds. We show that this conjecture is true for $n = 2$ and for some polytopes in higher dimensions.

7.12. Separating Codes and Traffic Monitoring

The paper [12] studies the problem of traffic monitoring which consists of differentiating a set of walks on a directed graph by placing sensors on as few arcs as possible. The problem of characterising a set of individuals by testing as few attributes as possible is already well-known, but traffic monitoring presents new challenges that the previous models of separation fall short from modelling such as taking into account the multiplicity and order of the arcs in a walk. We introduce a new and stronger model of separation based on languages that generalises the traffic monitoring problem. We study three subproblems with practical applications and develop methods to solve them by combining integer linear programming, separating codes and language theory.

8. Bilateral Contracts and Grants with Industry

8.1. Collaboration with EDF on robust maintenance planning

Our project with EDF concerns the optimization of the long term energy production planning, allowing for nuclear power plants maintenance. The challenges are to handle the large-scale instance of a five year planning and to handle the stochastic aspects of the problem: the stochastic variation of the electricity demand, the production capacity and the duration of maintenance period. The key decisions to be optimized are the dates of outages (for maintenance) and the level refuelling that determines the production of the year to come. We previously developed a column generation approach based on extended formulation which enables to solve within a few minutes a deterministic instance of the problem, which is within the time frame of the operational tools currently used by EDF. We now investigate stochastic and robust versions of the problem, where the duration of maintenance operations and the power demand are uncertain. Our approaches shall be evaluated on real life instances within a rolling horizon framework.

8.2. Collaboration with ERTUS on phytosanitary treatment planning

In planning winery operations (most importantly phytosanitary treatments on the wine tree) under weather forecast uncertainty, one searches for solutions that remain feasible and “cheap” in case of perturbation in the data. We consider the planning and scheduling of the operations that arise over a one-year horizon. More precisely, the operations to be scheduled include tasks related to soil care, or grape tree care: cutting, line building, thinning out leaves, ..., and chemical treatments. The latter are a main focus of our study since one of the principal goals of better planning is to reduce the amount of chemical treatments by selecting the appropriate products and schemes, but also by spacing out treatments while guaranteeing a disease free vineyard with some confidence. Each of the scheduled tasks requires its own resource, so the planning also triggers equipment and raw products selection decisions. The objective is to minimize both equipment and product costs augmented by an evaluation of the hazard of chemical product use. The planning should be “robust” to seasonal variations on the proper time frame for scheduling tasks.
8.3. Collaboration with St-Gobain Recherche on glass cutting

Through the PhD of Quentin Viaud, we study a hard glass-cutting problem. The objective is to minimize the quantity of trim loss when rectangular pieces are cut from large rectangles. This first study has shown that our methodologies are able to cope with this problem for medium-size instances. Solving the problem with large instances is a scientific challenge that we will address in the a follow-up contract.

8.4. Collaboration with SNCF on timetable and rolling stock rotation planning

Our project with SNCF concerns the optimisation of timetable and rolling stock rotation planning. The railway production planning process combines heterogeneous resources and is usually decomposed into different sequential sub-problems, beginning by line planning, timetabling, rolling stock rotations and crew scheduling. Our goal is to solve the timetable and rolling stock problems in an integrated manner. Given a line planning and service requirement constraints, the problem is to produce a timetable for a set of trains and the objective is to minimize the cost of the railcars used. An originality of our approach is to deal with railcars composed of multiple units, which can be coupled or decoupled at some stations. The PhD thesis of Mohamed Benkirane is funded by this project.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

9.1.1.1. ANR Solhar (ANR-13-MONU-0007)

This project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computing platforms equipped with accelerators. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool. The focus of RealOpt in this project is on the scheduling aspect. Indeed, executing a heterogeneous workload with complex dependencies on a heterogeneous architecture is a very challenging problem that demands the development of effective scheduling algorithms. These will be confronted with possibly limited views of dependencies among tasks and multiple, and potentially conflicting objectives, such as minimizing the makespan, maximizing the locality of data or, where it applies, minimizing the memory consumption.

See also: http://solhar.gforge.inria.fr/

9.2. International Initiatives

9.2.1. Inria International Partners

In the follow-up of our 6 year Inria Associate Team project SAMBA, we have set an important research collaboration with Brazil (Universidade Federal Fluminense, Pontificia Universidade Catolica do Rio de Janeiro) and Chile (Universidad Adolfo Ibanez). This results in joint publications and frequent visits, including long stay by research students.
9.3. International Research Visitors

9.3.1. Visits of International Scientists

- Teobaldo LEITE BULHOES, from Universidade Federal Fluminense (Niteroi, Brazil), visited the team from October 23rd to December 13th 2017.
- Orlando Rivera Letelier, from Universidad Adolfo Ibanez, Chile, visited the team for January 2017.
- Eduardo UCHOA, from Universidade Federal Fluminense (Niteroi, Brazil), visited the team during two weeks from November 5th to 18th 2017.
- Xuding ZHU, from Zhejiang Normal University (Jinhua, China) visited the team during one month in June 2017.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- Arnaud Pêcher, François Clautiaux and Pierre Pesneau have organized "Journées Graphes et Algorithmes", Bordeaux, November 15-17, 2017

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

- Olivier Beaumont is the Chair of the Algorithm Track of Super Computing 2017 (November, Denver, USA); "The International Conference for High Performance Computing, Networking, Storage and Analysis" [https://sc17.supercomputing.org](https://sc17.supercomputing.org)
- Lionel Eyraud-Dubois is Chair of the “Cloud Computing and Data Center Management” track of I-SPAN 2017; the 14th International Symposium on Pervasive Systems, Algorithms, and Networks

10.1.2.2. Member of the Conference Program Committees

The team members are members of the following program committees:

- Lionel Eyraud-Dubois and Olivier Beaumont: HiPC 2017: 24th IEEE International Conference on High Performance Computing, Data, and Analytics
- Lionel Eyraud-Dubois: REPPAR 2017: 4th International Workshop on Reproducibility in Parallel Computing
10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Olivier Beaumont is editor for IEEE Transactions on Parallel and Distributed Systems (TPDS)
- François Vanderbeck is Associate Editor for the EURO Journal on Computational Optimization
- François Clautiaux is Associate Editor for Mathematical Programming and Exact Methods in the journal ISTE “Recherche Opérationnelle”

10.1.3.2. Reviewer - Reviewing Activities

The team members are regular referees for the best journals of the field.

10.1.4. Invited Talks


10.1.5. Leadership within the Scientific Community

Our group is actively preparing the triennal symposium of the international mathematical optimization society. We organize it in Bordeaux in July 2018. 2000 attendees are expected.

10.1.6. Scientific Expertise

- Olivier Beaumont is a member of the INCITE (math-comp track) panel
- Olivier Beaumont is an expert for the H2020-FET-OPEN-2016 projects

10.1.7. Research Administration

- Olivier Beaumont is the scientific deputy of Inria Bordeaux Sud-Ouest and a member of the Evaluation Committee of Inria Verify it!!.
- François Vanderbeck is taking care of the team OptimAl (“Optimisation Mathématique Modèle Aléatoire et Statistique”) at the Mathematics Institute of Bordeaux.
- Arnaud Pêcher is the head of the Computer Science Department, IUT of Bordeaux.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Licence : A. Pêcher, Programmation Impérative, 10h, DUT, Université de Bordeaux, France
- Licence : A. Pêcher, Conception Objet, 42h, DUT, Université de Bordeaux, France
- Licence : A. Pêcher, Programmation objet en Java, 44h, DUT, Université de Bordeaux, France
- Licence : A. Pêcher, Algorithmique Avancée, 32h, DUT, Université de Bordeaux, France
- Licence : A. Pêcher, Assembleur, 24h, DUT, Université de Bordeaux, France
- Licence : A. Pêcher, Programmation Mobile, 24h, DUT, Université de Bordeaux, France
- Master : F. Clautiaux, Gestion des Opérations et Planification de la Production, 20h, M2, Université de Bordeaux, France
- Master : F. Clautiaux, Flot et Combinatoire, 10h, M2, Institut Polytechniques de Bordeaux, France
- Master : F. Clautiaux, Introduction à la Programmation en Variables Entières, 20h, M1, Université de Bordeaux, France
- Master : F. Clautiaux, Projet d’optimisation pour l’insertion professionnelle, M2, Université de Bordeaux, France
Master : L. Eyraud-Dubois, Optimisation en Cloud Computing et Big Data, 15h, M2, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Optimisation, 37h, L2, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Programmation pour le calcul scientifique, 24h, L2, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Recherche Opérationnelle, 24h, DUT, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Algorithmique et Programmation 1, 28h, M1, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Programmation linéaire, 29h, M1, Université de Bordeaux, France
Licence : Licence : P. Pesneau, Optimisation dans les graphes (partie flots), 15h, M1, Université de Bordeaux, France
Master : O. Beaumont, Approximation et Big Data, 15h, M2, Université de Bordeaux, France
Master : O. Beaumont, Distributed Computing and Data Mining, 4h, M2, Institut National Polytechnique de Bordeaux, France
Licence : B. Detienne, Initiation à l’ingénierie en optimisation, 12h, L1, Université de Bordeaux, France
Licence : B. Detienne, Modèles et Méthodes d’Optimisation, 21h, L2, Université de Bordeaux, France
Licence : B. Detienne, Groupe de travail applicatif, 12h, L3, Université de Bordeaux, France
Master : B. Detienne, Optimisation continue, 43h, M1, Université de Bordeaux, France
Master : B. Detienne, Problèmes combinatoires et routage, 14h, M1, Université de Bordeaux, France
Master : B. Detienne, Problèmes combinatoires et routage, 14h, M1, Institut National Polytechnique de Bordeaux, France
Master : B. Detienne, Optimisation dans l’incertain, 58h, M2, Université de Bordeaux, France
Master : R. Sadykov, Introduction à la Programmation par Contraintes, 30h, M1, Université de Bordeaux, France
Master : I. Tahiri, Recherche Opérationnelle, 16h, M1, Institut National Polytechnique de Bordeaux, France
Master : F. Vanderbeck, Recherche Opérationnelle, 15h, M1, Institut National Polytechnique de Bordeaux, France
Master : F. Vanderbeck, Programmation Entière, 58h, M2, Université de Bordeaux, France

10.2.2. Supervision

PhD : Suraj Kumar, Scheduling of Dense Linear Algebra Kernels on Heterogeneous Resources [10], Université de Bordeaux, 12/04/2017, Olivier Beaumont (dir) and Lionel Eyraud-Dubois (co-dir)
PhD : Thomas Lambert, Placement de tâches et réplication de fichiers sur plates-formes parallèles [11], Université de Bordeaux, 8/09/2017, Olivier Beaumont (dir) and Lionel Eyraud-Dubois (co-dir)
PhD in progress : Jérémy Guillot, Optimisation de problèmes de partitionnement, from September 2014, François Clautiaux (dir) and Pierre Pesneau (dir).
PhD in progress : Quentin Viaud, Méthodes de programmation mathématiques pour des problèmes complexes de découpe, from January 2015, François Clautiaux (dir), Ruslan Sadykov (dir), and François Vanderbeck (co-dir).
PhD in progress: Rodolphe Griset, Robust planning in Electricity production, from November 2015, Boris Detienne (dir) and François Vanderbeck (dir).

PhD in progress: Imen Ben Mohamed, Location routing problems, from October 2015, Walid Klibi (dir) and François Vanderbeck (dir).

PhD in progress: Thomas Bellitto, Infinite graphs, from September 2015, Arnaud Pécher (dir) and Christine Bachoc (dir).

PhD in progress: Guillaume Marques, Planification de tournées de véhicules avec transbordement en logistique urbaine: approches basées sur les méthodes exactes de l’optimisation mathématique, from September 2017, François Vanderbeck (dir) and Ruslan Sadykov (co-dir).

PhD in progress: Gaël Guillot, Aggregation and disaggregation methods for hard combinatorial problems, from November 2017, François Clautiaux (dir) and Boris Detienne (dir).

10.2.3. Juries

- Lionel Eyraud-Dubois participated in the jury of Raphaël Bleuse, who defended on October 11, 2017, at Université de Grenoble Alpes.
- Olivier Beaumont: Evaluation (rapporteur) and President of the PhD thesis committee of Aymen Jlassi (University of Tours, France).
- Olivier Beaumont: Member of the PhD thesis committee of Alexandre Perrot (University of Bordeaux, France).
- Olivier Beaumont: Member of the PhD thesis committee of Noel Gillet (University of Bordeaux, France).
- François Vanderbeck: Member of the PhD thesis committee of Nicolas HUIN (Inria Sophia)

10.3. Popularization

- François Clautiaux is a member of the board of AMIES, the French Agency for Interaction in Mathematics with Business and Society. AMIES is a national organization that aims to develop relations between academic research teams in mathematics and business, especially SMEs.
- Olivier Beaumont participated to “Unithé ou Café” (May 19, 2017), a local event dedicated to popular science on the topic of online algorithms.
- Olivier Beaumont participated to “La Fête de la Science” (October 3 and 4, 2017) on the computation of PageRank.

11. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


Invited Conferences


International Conferences with Proceedings


National Conferences with Proceeding


Conferences without Proceedings


[29] G. GUILLOT, F. CLAUTIAUX, B. DETIENNE. Une méthode basée sur la programmation dynamique pour résoudre le problème de sac à dos temporel, in "Dixièmes Journées Polyèdres et Optimisation Combinatoire JPOC10". Paris, France, June 2017, https://hal.inria.fr/hal-01670226.


Research Reports


[34] O. BEAUMONT, T. LAMBERT, L. MARCHAL, B. THOMAS. Matching-Based Assignment Strategies for Improving Data Locality of Map Tasks in MapReduce, Inria - Research Centre Grenoble – Rhône-Alpes ; Inria Bordeaux Sud-Ouest, February 2017, nº RR-8968, https://hal.inria.fr/hal-01386539.


[37] R. SADYKOV, E. UCHOA, A. ALVES PESSOA. A Bucket Graph Based Labeling Algorithm with Application to Vehicle Routing, Universidade Federal Fluminense, October 2017, nº Cadernos do LOGIS 2017/7, https://hal.inria.fr/hal-01664854.

Other Publications

[38] G. AUPY, O. BEAUMONT, L. EYRAUD-DUBOIS. What size should your Burst-Buffers be?, October 2017, working paper or preprint, https://hal.inria.fr/hal-01623846.
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Project-Team SISTM

Statistics In System biology and Translational Medicine

IN PARTNERSHIP WITH:
INSERM
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences
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10. **Dissemination**

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

10.1.2.2. Member of the Conference Program Committees

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

10.1.3.2. Reviewer - Reviewing Activities

10.1.4. Invited Talks

10.1.5. Leadership within the Scientific Community

10.1.6. Scientific Expertise

10.1.7. Research Administration

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

10.2.2. Supervision

10.2.3. Juries

10.3. Popularization

11. **Bibliography**
Project-Team SISTM

Creation of the Team: 2013 April 02, updated into Project-Team: 2015 January 01

Keywords:

**Computer Science and Digital Science:**
- A3.3.2. - Data mining
- A3.3.3. - Big data analysis
- A3.4.1. - Supervised learning
- A3.4.2. - Unsupervised learning
- A3.4.4. - Optimization and learning
- A3.4.5. - Bayesian methods
- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.2.4. - Statistical methods
- A6.3.1. - Inverse problems
- A6.3.4. - Model reduction
- A6.4.2. - Stochastic control

**Other Research Topics and Application Domains:**
- B1.1. - Biology
- B1.1.6. - Genomics
- B1.1.7. - Immunology
- B1.1.9. - Bioinformatics
- B1.1.11. - Systems biology
- B1.1.14. - Microbiology
- B2.2.4. - Infectious diseases, Virology
- B2.2.5. - Immune system diseases
- B2.3. - Epidemiology
- B2.4.1. - Pharmacokinetics and dynamics
- B2.4.2. - Drug resistance

1. Personnel

**Research Scientists**
- Daniel Commenges [Inserm, Senior Researcher, HDR]
- Mélanie Prague [Inria, Researcher]

**Faculty Members**
- Rodolphe Thiébaut [Team leader, Univ.de Bordeaux, Professor, PUPH, HDR]
- Marta Avalos Fernandez [Univ Bordeaux, Associate Professor]
- Robin Genuer [Univ Bordeaux, Associate Professor]
- Boris Hejblum [Univ Bordeaux, Associate Professor]
- Laura Richert [Univ Bordeaux, Associate Professor, MCUPH]

**Technical Staff**
- Henri Bonnabau [Univ Bordeaux]
- Chariff Alkhassim [Inserm]
2. Overall Objectives

2.1. Overall Theoretical Objectives

The overall objective of SISTM is to develop statistical methods for the integrative analysis of health data, especially those related to clinical immunology to answer specific questions risen in the application field. To reach this objective we are developing statistical methods belonging to two main research areas:

- Statistical and mechanistic modeling, especially based on ordinary differential equation systems, fitted to population and sparse data
- Statistical learning methods in the context of high-dimensional data

These two approaches are used for addressing different types of questions. Statistical learning methods are developed and applied to deal with the high dimensional characteristics of the data. The outcome of this research leads to hypotheses linked to a restricted number of markers. Mechanistic models are then developed and used for modeling the dynamics of a few markers. For example, regularized methods can be used to select relevant genes among 20000 measured with microarray technology, whereas differential equations can be used to capture the dynamics and relationship between several genes followed over time by a q-PCR assay or RNA-seq.

2.2. Overall Applied Objectives

Data are generated in clinical trials or biological experimentation. Our main application of interest is the immune response to vaccine or other immune interventions (such as exogenous cytokines), mainly in the context of HIV infection. The methods developed in this context can be applied in other circumstances but the focus of the team on immunology is important for the relevance of the results and their translation into practice, thanks to a longstanding collaboration with several immunologists and the implication of the team in the Labex Vaccine Research Institute (http://vaccine-research-institute.fr). Examples of objectives related to this application field are:

- To understand how immune response is generated with immune interventions (vaccines or interleukines)
- To predict what would be the immune response to a given immune intervention for designing next studies and adapting interventions to individual patients
3. Research Program

3.1. Mecanistic modelling

When studying the dynamics of a given marker, say the HIV concentration in the blood (HIV viral load), one can for instance use descriptive models summarising the dynamics over time in term of slopes of the trajectories [57]. These slopes can be compared between treatment groups or according to patients’ characteristics. Another way for analysing these data is to define a mathematical model based on the biological knowledge of what drives HIV dynamics. In this case, it is mainly the availability of target cells (the CD4+ T lymphocytes), the production and death rates of infected cells and the clearance of the viral particles that impact the dynamics. Then, a mathematical model most often based on ordinary differential equations (ODE) can be written [50]. Estimating the parameters of this model to fit observed HIV viral load gave a crucial insight in HIV pathogenesis as it revealed the very short half-life of the virions and infected cells and therefore a very high turnover of the virus, making mutations a very frequent event [49].

Having a good mechanistic model in a biomedical context such as HIV infection opens doors to various applications beyond a good understanding of the data. Global and individual predictions can be excellent because of the external validity of a model based on main biological mechanisms. Control theory may serve for defining optimal interventions or optimal designs to evaluate new interventions [42]. Finally, these models can capture explicitly the complex relationship between several processes that change over time and may therefore challenge other proposed approaches such as marginal structural models to deal with causal associations in epidemiology [41].

Therefore, we postulate that this type of model could be very useful in the context of our research that is in complex biological systems. The definition of the model needs to identify the parameter values that fit the data. In clinical research this is challenging because data are sparse, and often unbalanced, coming from populations of subjects. A substantial inter-individual variability is always present and needs to be accounted as this is the main source of information. Although many approaches have been developed to estimate the parameters of non-linear mixed models [53], [60], [45], [51], [46], [59], the difficulty associated with the complexity of ODE models and the sparsity of the data leading to identifiability issues need further research.

3.2. High dimensional data

With the availability of omics data such as genomics (DNA), transcriptomics (RNA) or proteomics (proteins), but also other types of data, such as those arising from the combination of large observational databases (e.g. in pharmacoepidemiology or environmental epidemiology), high-dimensional data have become increasingly common. Use of molecular biological technics such as Polymerase Chain Reaction (PCR) allows for amplification of DNA or RNA sequences. Nowadays, microarray and Next Generation Sequencing (NGS) techniques give the possibility to explore very large portions of the genome. Furthermore, other assays have also evolved, and traditional measures such as cytometry or imaging have became new sources of big data. Therefore, in the context of HIV research, the dimension of the datasets has much grown in term of number of variables per individual than in term of number of included patients although this latter is also growing thanks to the multi-cohort collaborations such as CASCADE or COHERE organized in the EuroCoord network⁰. As an example, in a recent phase 1/2 clinical trial evaluating the safety and the immunological response to a dendritic cell-based HIV vaccine, 19 infected patients were included. Bringing together data on cell count, cytokine production, gene expression and viral genome change led to a 20 Go database [56]. This is far from big databases faced in other areas but constitutes a revolution in clinical research where clinical trials of hundred of patients sized few hundred of Ko at most. Therefore, more than the storage and calculation capacities, the challenge is the comprehensive analysis of these datasets.

⁰see online at http://www.eurocoord.net
The objective is either to select the relevant information or to summarize it for understanding or prediction purposes. When dealing with high dimensional data, the methodological challenge arises from the fact that datasets typically contain many variables, much more than observations. Hence, multiple testing is an obvious issue that needs to be taken into account [54]. Furthermore, conventional methods, such as linear models, are inefficient and most of the time even inapplicable. Specific methods have been developed, often derived from the machine learning field, such as regularization methods [58]. The integrative analysis of large datasets is challenging. For instance, one may want to look at the correlation between two large scale matrices composed by the transcriptome in the one hand and the proteome on the other hand [47]. The comprehensive analysis of these large datasets concerning several levels from molecular pathways to clinical response of a population of patients needs specific approaches and a very close collaboration with the providers of data that is the immunologists, the virologists, the clinicians...

4. Application Domains

4.1. Systems Biology and Translational medicine

Biological and clinical researches have dramatically changed because of the technological advances, leading to the possibility of measuring much more biological quantities than previously. Clinical research studies can include now traditional measurements such as clinical status, but also thousands of cell populations, peptides, gene expressions for a given patient. This has facilitated the transfer of knowledge from basic to clinical science (from “bench side to bedside”) and vice versa, a process often called ”Translational medicine”. However, the analysis of these large amounts of data needs specific methods, especially when one wants to have a global understanding of the information inherent to complex systems through an “integrative analysis”. These systems like the immune system are complex because of many interactions within and between many levels (inside cells, between cells, in different tissues, in various species). This has led to a new field called "Systems biology" rapidly adapted to specific topics such as "Systems Immunology" [55], "Systems vaccinology" [52], "Systems medicine" [44]. From the statistician point of view, two main challenges appear: i) to deal with the massive amount of data ii) to find relevant models capturing observed behaviors.

4.2. The case of HIV immunology

The management of HIV infected patients and the control of the epidemics have been revolutionized by the availability of highly active antiretroviral therapies. Patients treated by these combinations of antiretrovirals have most often undetectable viral loads with an immune reconstitution leading to a survival which is nearly the same to uninfected individuals [48]. Hence, it has been demonstrated that early start of antiretroviral treatments may be good for individual patients as well as for the control of the HIV epidemics (by reducing the transmission from infected people) [43]. However, the implementation of such strategy is difficult especially in developing countries. Some HIV infected individuals do not tolerate antiretroviral regimen or did not reconstitute their immune system. Therefore, vaccine and other immune interventions are required. Many vaccine candidates as well as other immune interventions (IL7, IL15) are currently evaluated. The challenges here are multiple because the effects of these interventions on the immune system are not fully understood, there are no good surrogate markers although the number of measured markers has exponentially increased. Hence, HIV clinical epidemiology has also entered in the era of Big Data because of the very deep evaluation at individual level leading to a huge amount of complex data, repeated over time, even in clinical trials that includes a small number of subjects.

4.3. The case of Ebola vaccine development

In response to the recent outbreak of Ebola virus disease in West Africa, the clinical development of some candidate to Ebola vaccine has been accelerated. Several vectors, mostly encoding glycoprotein of the virus, were tested in Phase I-II studies in order to assess their safety and immunogenicity. One of the main question of interest there is the antibody response induced by vaccination, as some non-human primates studies have
shown protection against the virus when antibody levels were high enough. Although bridging studies still have to be developed, antibodies are thus considered as a criterium of interest. The challenge is then to evaluate the durability of the antibody response, whether it be at an individual or population level, in order to evaluate the impact of a vaccine strategy in case of an epidemic. Moreover, we are interested in the factors associated to this antibody response, and even more the other immune markers (from both innate and adaptative immune response) able to predict antibody levels. As those relationship are non-linear, sophisticated statistical and mathematical methods are developed in order to address these questions. A systems medicine approach using multidimensional immunogenicity data from clinical trials and statistical models can help to understand vaccine mechanisms and improve the selection of optimised vaccine strategies for clinical trials.

5. Highlights of the Year

5.1. Highlights of the Year

Funding by PIA3 of the Bordeaux Graduate’s School in Digital Public Health, headed by Rodolphe Thiébaut. This Master/PhD program is built with the expertise coming from the Inria Sistm project team and in collaboration with several other teams (MONC, CARMEN, PHOENIX).

Successful application of integrative analyses tools on high dimensional immunogenicity data from an Ebola vaccine trial with identification of early correlates of later antibody responses [30]

We published a milestone paper in Biometrics comparing descriptive models (Marginal structural models) and mechanistic models (Ordinary differential equations with mixed effect models on parameters). This is impactful as it shows that mechanistic models can adequately estimate a treatment effect in time-varying confounders settings as it is in observational studies. This opens the perspective of in silico trials based on predictions based on the analysis of available cohorts. [26]

We published a robust and powerful statistical method to analyzed longitudinal RNAseq data, largely outperforming state-of-the-art methods. With the surge in RNAseq data production, e.g. in system vaccinology, this principled methodology has a broad impact in deepening our understanding of underlying molecular mechanisms in various contexts, paving the way for further biological innovation. [16]

5.1.1. Awards

The University of Bordeaux Initiative of Excellence (IdEx) and Zellidja travel grants for a research PhD student visit of 3 months to the CSIRO’s machine learning Data61 team, Canberra, Australia (Perrine Soret).

6. New Software and Platforms

6.1. marqLevAlg

Keywords: Optimization - Biostatistics

Functional Description: An R package for function optimization. Available on CRAN, this package performs a minimization of function based on the Marquardt-Levenberg algorithm. This package is really useful when the surface to optimize is non-strictly convex or far from a quadratic function. A new convergence criterion, the relative distance to maximum (RDM), allows the user to have a better confidence in the stopping points, other than basic algorithm stabilization.

- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/marqLevAlg/index.html

6.2. VSURF

Variable Selection Using Random Forests
FUNCTIONAL DESCRIPTION: An R package for Variable Selection Using Random Forests. Available on CRAN, this package performs an automatic (meaning completely data-driven) variable selection procedure. Originally designed to deal with high dimensional data, it can also be applied to standard datasets.

- Contact: Robin Genuer
- URL: https://github.com/robingenuer/VSURF

6.3. NPflow

Bayesian Nonparametrics for Automatic Gating of Flow-Cytometry Data

FUNCTIONAL DESCRIPTION: Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data pre-processing applications.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/NPflow/

6.4. COVVSURF

Combination of Clustering Of Variables and Variable Selection Using Random Forests

FUNCTIONAL DESCRIPTION: R package to fit a sequence of conditional logistic regression models with lasso, for small to large sized samples.

- Partner: DRUGS-SAFE
- Contact: Marta Avalos Fernandez
- URL: https://cran.r-project.org/web/packages/clogitLasso/index.html

6.5. clogitLasso

FUNCTIONAL DESCRIPTION: An R package for the gene set analysis of longitudinal gene expression data sets. This package implements a Time-course Gene Set Analysis method and provides useful plotting functions facilitating the interpretation of the results.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/TcGSA/index.html

6.6. TcGSA

FUNCTIONAL DESCRIPTION: We have written a specific program called NIMROD for estimating parameter of ODE based population models.

- Contact: Melanie Prague
6.8. tcgsaseq

Time-Course Gene Set Analysis for RNA-Seq Data

KEYWORDS: Genomics - Biostatistics - Statistical modeling - RNA-seq - Gene Set Analysis

FUNCTIONAL DESCRIPTION: Gene set analysis of longitudinal RNA-seq data with variance component score test accounting for data heteroscedasticity through precision weights.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/tcgsaseq/index.html

6.9. cytometree

KEYWORDS: Clustering - Biostatistics - Bioinformatics

FUNCTIONAL DESCRIPTION: Given the hypothesis of a bimodal distribution of cells for each marker, the algorithm constructs a binary tree, the nodes of which are subpopulations of cells. At each node, observed cells and markers are modeled by both a family of normal distributions and a family of bimodal normal mixture distributions. Splitting is done according to a normalized difference of AIC between the two families.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/cytometree/index.html

6.10. CRTgeeDR

KEYWORDS: Missing data - Statistics - Regression

FUNCTIONAL DESCRIPTION: The CRTgeeDR package allows you to estimate parameters in a regression model (with possibly a link function). It allows treatment augmentation and IPW for missing outcome. It is particularly of use when the goal is to estimate the intervention effect of a prevention strategy against epidemics in cluster randomised trials.

- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/CRTgeeDR/index.html

6.11. ludic

KEYWORDS: Probability - Biostatistics

FUNCTIONAL DESCRIPTION: An R package to perform probabilistic record Linkage Using only Dlagnosis Codes without direct identifiers, using C++ code to speed up computations. Available on CRAN, development version on github.

- Contact: Boris Hejblum
- URL: https://cran.r-project.org/web/packages/ludic/index.html
7. New Results

7.1. Statistical and mechanistic modeling

  Comparison of descriptive models (Marginal structural models) and mechanistic models (Ordinary differential equations with mixed effect models on parameters) performances for estimating treatment effect from observational studies.


  Review of the literature on how to analyse data from a cluster randomised trial

  Modelling the disability of CD4 restoration by repeated cycles of Interukine-7 injections using mechanistic models.

  Doubly robust approach to estimate the treatment effect in Cluster randomised trials.

7.2. Statistical learning methods for high-dimensional data

  Addresses the analysis of Big Data with Random Forests, review of existing algorithms, simulation study and recommendations.

  We propose tcgsaseq, a principled, model-free, and efficient method for detecting longitudinal changes in RNA-seq gene sets defined a priori. Applied to both simulated data and two real datasets, tcgsaseq is shown to exhibit very good statistical properties, with an increase in stability and power when compared to state-of-the-art methods

  We propose to use a Bayesian nonparametric approach with Dirichlet process mixture of multivariate skew t-distributions to perform model based clustering of flow-cytometry data, robustly estimating the number of cell populations from the data.

7.3. Software tools
  This is a review on the methods to visualize the big data in the context of clinical research.
  Diffusion of a package to estimate estimate the intervention effect of a prevention strategy against epidemics in cluster randomised trials. Estimation is based on GEE.

7.4. Analysis of results from Clinical trials and cohorts in HIV
  This is a tool that should help clinicians to evaluate the immunological response to antiretroviral therapy in HIV infected patients. Thanks to the analyse of one of the largest observational database in the world, we provide with an online tool references on the CD4 count during the first year of antiretroviral therapy.
  This is an analysis of data on gene expression and factors associated to the immune activation in HIV-infected patients. Using structural models, we disentangle the effect of factors such as CMV and the mediation through type 1 interferon pathway.
  In this work, we have demonstrated the independent effect of the biomarker ST2 on the overall mortality in a large cohort of HIV infected patients.
• Vladimir Novitsky, Mélanie Prague, Sikhulile Moyo, Tendani Gaolathe, Mompati Mmalane, et al.. High HIV-1 RNA among Newly Diagnosed People in Botswana. AIDS Research and Human Retroviruses, Mary Ann Liebert, To appear.

7.5. Analysis of results from Clinical trials and cohorts in Ebola
  In this work, we have analyzed high-dimensional gene expression and cell characterization data. We showed the predictive capacity of the innate immune response to the Ebola vaccine to define the antibody response established beyond one month. This is a successful application of integrative analyses tools on high dimensional immunogenicity data from an Ebola vaccine trial with identification of early correlates of later antibody responses.
7.6. Analysis of results from clinical trials and cohorts in other fields
(Epidemiology, Medical Sciences, Neuroimaging, Sport Sciences)

  Joint work with the GIN-IMN team, application of a variable selection procedure based on SVM method to analyze functional MRI data.

  Application of Multiple Correspondence Analysis which enlights frailty and dependent profile of people from the Three-city study.

  Exploration of the association between the use of medicinal drugs and the risk of being involved in a road traffic crash as a pedestrian. We applied the Lasso methodology that we previously developed for the case-crossover design in a high-dimensional setting. This design controls for time-invariant factors by using each case as its own control. This study highlights the necessity of improving awareness of the effect of medicines on pedestrians.

  Quantification of the relationships between the effects of periodization variables and competitive performance in elite swimmers using semiparametric mixed effects models. In the framework of the 2014-2016 R&D project "Quels schémas de périodisation pour la préparation des Jeux Olympiques à Rio ?" with the French Swimming Federation.

  We show that anti-cit-fibrinogen antibodies as a group were associated with CAD outcomes in our RA cohort, with the strongest signal for association arising from a subset of the autoantibodies.

  We demonstrated application of a bioinformatics method, the PheWAS, to screen for the clinical significance of RA-related autoantibodies. Using the PheWAS approach, we identified potentially significant links between variations in the levels of autoantibodies and comorbidities of interest in RA.

7.7. Conferences

Members of the team were involved in 12 talks during conferences and colloquium.

Mélanie Prague has her work presented in 2017 in 2 peer-reviewed international conferences (Society of clinical trials Liverpool UK and Keystone symposium of mathematical modeling of virus infection, Este Park, May 2017).

Robin Genuer presented his work in the peer-reviewed International Conference of the European Research Consortium for Informatics and Mathematics Working Group (ERCIM WG) on Computational and Methodological Statistics, University of London, UK.
Boris Hejblum presented his work in the peer-reviewed 38th Annual Conference of the International Society for Clinical Biostatistics.
Chloé Pasin presented her work in the peer-reviewed Systems Immunology & Vaccine Design symposium, Heidelberg, Germany and the French Applied and Industrial Mathematics Society (SMAI) conference (Roncelles-Bains).
Members of the team participated in French conferences: GDR Stat santé Bordeaux, GDR mathematical modelling of life Lyon and Journées de la statistique Francaise, Avignon (Perrine Soret, Mélanie Prague, Boris Hejblum). Mélanie Prague and Boris Hejblum also presented 4 posters in workshops.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Implication in research for the development of vaccine has lead to a direct contracts with industry such Iliad Biotechnologies. This contract had been signed for the BPZE-1 pertussis vaccine trial. This study evaluates the safety and immunogenicity of a higher dose formulation of a new live attenuated vaccine, BPZE1, intended to prevent Bordetella pertussis nasopharyngeal colonization and pertussis disease, and investigates whether higher doses of BPZE1 induce the live vaccine to colonize subjects’ nasopharynx. The study is a Phase Ib (high dose), single centre, dose-escalating, placebo-controlled study of the live attenuated B. pertussis strain BPZE1 given as a single intranasal dose to healthy adult volunteer.

8.2. Bilateral Grants with Industry

Implication in research for the development of Ebola vaccine has lead to several indirect contracts with industry:

- The EBOVAC1, EBOVAC2 and EBOVAC3 project, collaboration with Janssen from Johnson et Johnson.
- The BPZE-1 pertussis vaccine trial, which is presented in Section 'Bilateral Contracts with Industry', leads to collaboration with Iliad Biotechnologies.
- The Prevac trial vaccine trial leads to collaboration with Merck and Janssen. The purpose of this study is to evaluate the safety and immunogenicity of three vaccine strategies that may prevent Ebola virus disease (EVD) events in children and adults. Participants will receive either the Ad26.ZEBOV (rHAd26) vaccine with a MVA-BN-Filo (MVA) boost, or the rVSVΔG-ZEBOV-GP (rVSV) vaccine with or without boosting, or placebo.

9. Partnerships and Cooperations

9.1. Regional Initiatives

The team have strong links with:

- Research teams of the research center INSERM U1219 : "Injury Epidemiology, Transport, Occupation" (IETO), "Biostatistics", "Pharmacoepidemiology and population impact of drugs", "Multimorbidity and public health in patients with HIV or Hepatitis" (MORPH3Eus), "Computer research applied to health" (ERIAS) emerging research team.
- Bordeaux and Limoges CHU ("Centre Hospitalier Universitaire").
- Institut Bergonié, Univ Bordeaux through the Euclid platform.
- Inria Project-team MONC and CQFD.
The project team members are involved in:

- EUCLID/F-CRIN clinical trials platform (Laura Richert)
- The research project “Self-management of injury risk and decision support systems based on predictive computer modelling. Development, implementation and evaluation in the MAVIE cohort study” funded by the Nouvelle-Aquitaine regional council (Marta Avalos).
- Phenotyping from Electronic Health Records pilot project in cooperation with the ERIAS Inserm emerging team in Bordeaux and the Rheumatology service from the Bordeaux Hospital (Boris Hejblum)

9.2. National Initiatives

9.2.1. Labex Vaccine Research Institute (VRI)

There are strong collaborations with immunologists involved in the Labex Vaccine Research Institute (VRI) as Rodolphe Thiébaut is leading the Biostatistics/Bioinformatics division http://vaccine-research-institute.fr. Collaboration with Inserm PRC (pôle Recherche clinique).

9.2.2. Expert Appraisals

- Rodolphe Thiébaut is an expert for INCA (Institut National du Cancer) for the PHRC (Programme hospitalier de recherche Clinique en cancérologie) and for the PRME (Programme de recherche médico-économique en cancérologie).
- Rodolphe Thiébaut is a member of the CNU 46.04 (Biostatistiques, informatique médicale et technologies de communication).
- Rodolphe Thiébaut is a member of the Scientific Council of INSERM.
- Mélanie Prague is an expert for ANRS (France Recherche Nord&Sud Sida-HIV Hépatites) in the CSS 3 (Recherches cliniques et physiopathologiques dans l’infection à VIH).
- Laura Richert is an expert for the PHRC (Programme hospitalier de recherche Clinique).
- Marta Avalos is an expert for L’ANSM (Agence nationale de sécurité du médicament et des produits de santé)

9.2.3. Various Partnership

The project team members are involved in:

- DRUGS-SAFE platform funded by ANSM (Marta Avalos).
- F-CRIN (French clinical research infrastructure network) was initiated in 2012 by ANR under two sources of founding "INBS/Infrastructures nationales en biologie et en santé" and "Programme des Investissements d’avenir". (Laura Richert)
- I-REIVAC is the French vaccine research network. This network is part of the “Consortium de Recherche en Vaccinologie (CoReVac)” created by the “Institut de Microbiologie et des Maladies Infectieuses (IMMI)”. (Laura Richert)
- INCA (Institut National du Cancer) funded the project « Evaluation de l’efficacité d’un traitement sur l’évolution de la taille tumoraire et autres critères de survie : développement de modèles conjoints. » (Principal PI Virginie Rondeau Inserm U1219, Mélanie Prague is responsible of Work package 4 mechanistic modeling of cancer: 5800 euros).
- Contrat Initiation ANRS MoDeL-CI: Modeling the HIV epidemic in Ivory Coast (Principal PI Eric Ouattara Inserm U1219 in collaboration with University College London, Mélanie Prague is listed as a collaborator).
9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

The members of SISTM Team are involved in EHV A (European HIV Vaccine Alliance):

Program: Most information about this program can be found at http://www.ehv-a.eu.
Coordinator: Rodolphe Thiébaut is Work Package leader of the WP10 "Data Integration".
Other partners: The EHV A encompasses 39 partners, each with the expertise to promote a comprehensive approach to the development of an effective HIV vaccine. The international alliance, which includes academic and industrial research partners from all over Europe, as well as sub-Saharan Africa and North America, will work to discover and progress novel vaccine candidates through the clinic.

Abstract: With 37 million people living with HIV worldwide, and over 2 million new infections diagnosed each year, an effective vaccine is regarded as the most potent public health strategy for addressing the pandemic. Despite the many advances in the understanding, treatment and prevention of HIV made over the past 30 years, the development of broadly-effective HIV vaccine has remained unachievable. EHV A plans to develop and implement:

Discovery Platform with the goal of generating novel vaccine candidates inducing potent neutralizing and non-neutralizing antibody responses and T-cell responses
Immune Profiling Platform with the goal of ranking novel and existing (benchmark) vaccine candidates on the basis of the immune profile
Data Management/Integration/Down-Selection Platform, with the goal of providing statistical tools for the analysis and interpretation of complex data and algorithms for the efficient selection of vaccines
Clinical Trials Platform with the goal of accelerating the clinical development of novel vaccines and the early prediction of vaccine failure.

The members of SISTM Team and particularly Laura Richert are also involved in other H2020 projects such as SenseCog, Medit’aging and Orthunion.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

Program: The EBOVAC2 project is one of 8 projects funded under IMI Ebola+ programme that was launched in response to the Ebola virus disease outbreak. The project aims to assess the safety and efficacy of a novel prime boost preventive vaccine regimen against Ebola Virus Disease (EVD).
Project acronym: EBOVAC2
Project title: EBOVAC2
Coordinator: Rodolphe Thiébaut
Other partners: Inserm (France), Labex VRI (France), Janssen Pharmaceutical Companies of Johnson & Johnson, London School of Hygiene & Tropical Medicine (United Kingdom), The Chancellor, Masters and Scholars of the University of Oxford (United Kingdom), Le Centre Muraz (Burkina Faso), Inserm Transfert (France)

Abstract: Given the urgent need for an preventive Ebola vaccine strategy in the context of the current epidemic, the clinical development plan follows an expedited scheme, aiming at starting a Phase 2B large scale safety and immunogenicity study as soon as possible while assuring the safety of the trial participants.

Phase 1 trials to assess the safety and immunogenicity data of the candidate prime-boost regimen in healthy volunteers are ongoing in the UK, the US and Kenya and Uganda. A further study site has been approved to start in Tanzania. Both prime-boost combinations (Ad26.ZEBOV prime + MVA-BN-Filo boost; and MVA-BN-Filo prime + Ad26.ZEBOV boost) administered at different intervals are being tested in these trials.
Phase 2 trials (this project) are planned to start as soon as the post-prime safety and immunogenicity data from the UK Phase I are available. Phase 2 trials will be conducted in healthy volunteers in Europe (France and UK) and non-epidemic African countries (to be determined). HIV positive adults will also be vaccinated in African countries. The rationale for inclusion of European volunteers in Phase 2, in addition to the trials in Africa, is to allow for higher sensitivity in safety signal detection in populations with low incidence of febrile illnesses, to generate negative control specimens for assay development, to allow for inclusion of health care workers or military personnel that may be deployed to Ebola-endemic regions.

9.3.3. Collaborations with Major European Organizations

University of Oxford;
London School of Hygiene and Tropical Medicine;
University Hospital Hamburg;
Heinrich Pette Institute for Experimental Virology, Hambourg;
MRC, University College London

9.4. International Initiatives

9.4.1. Inria International Labs

Fred Hutchinson Cancer center, Seattle;
Baylor Institute for Immunology (Dallas);
Duke University;
Collaborations through clinical trials: NIH for the Prevac trial, NGO Alima for the Prevac trial, Several African clinical sites for Ebovac2 and Prevac trials;
NIH program project grant "Revealing Reservoirs During Rebound", Harvard School of Public Health (HSPH) and the University of California, San Diego (P01AI131385, total budget $1.5M/yr for 5 years starting Oct 2017, both university manage the funding. Mélanie Prague is part of modelling unit of the "Quantitative Methods" research project (budget $220,000/yr). The principal investigator for this core is Victor de Grutolla (HSPH) The overall goal of this grant is to characterize viral rebound following antiretroviral therapy cessation in cohorts of patients who have started therapy early in infection, as well as in a cohort of terminally-ill patients who will interrupt therapy before death and subsequently donate their bodies to research.
Project submitted by the Inria DYNAMO-HIVE team with the laboratory “Program for evolutionary Dynamics” at Harvard (head Martin Nowak).
Denis Agniel from the RAND Corporation on developing statistical methods for the analysis of RNA-seq data (Boris Hejblum).
Tianxi Cai from Harvard University on developing methods for the linkage and analysis of Electronic Health Records data (Boris Hejblum).
Katherine Liao from Harvard University on the analysis of Electronic Health Records data in the context of Rheumatoid Arthritis (Boris Hejblum).
Machine learning team Data61 at CSIRO, Australia

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Alison Hill from “Program for evolutionary Dynamics” at Harvard visited the SISTM team twice (each time for 5 days) in May 2017 and July 2017. Main topic discussed was mechanistic modelling of new agents in HIV cure.
Linda Valeri from “Harvard medical school” visited the SISTM team 3 days. Main topic discussed was mediation analysis in high dimension.
Denis Agniel (RAND Corporation) visited B. Hejblum in Bordeaux for a week in May for a research collaboration
Visiting PhD student from Marcus Altfeld’s team: Annika Niehrs (2 week stay with SISTM).

9.5.2. Visits to International Teams
Marta Avalos visited David Conesa 1 week in October through the Erasmus+ program Universidad de Valencia (Espagne).
Mélanie Prague got invited in University of Pennsylvania (Philadelphia) for a 2-days research trip in the Biostatistics department on April 2-3 2017.
Mélanie Prague spend 10 days in Boston as an invited researcher in Harvard School of Public Health, Biostatistics department on April 10-15 2017.
Boris Hejblum visited Harvard University for a week in November 2017 for a research collaboration with Katherine Liao & Tianxi Cai.

9.5.2.1. Research Stays Abroad
Marta Avalos was a research visitor at CSIRO’s Data61 in Canberra, Australia from Dec. 2016 until June 2017. Collaboration with Cheng Soon Ong http://www.ong-home.my/
Perrine Soret was a research student visitor at CSIRO’s Data61 in Canberra (Australia) from Feb. 2017 to April 2017. Collaboration with Cheng Soon Ong. Funding: The University of Bordeaux Initiative of Excellence and Zellidja travel grants for a research visit of 3 months.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees
Daniel Commenges co-organised a SFB (French Region of the International Biometric Society) and GdR ”Statistique et Santé” conference in Bordeaux (http://gdr-stat-sante.math.cnrs.fr/spip/spip.php?rubrique20),
Daniel Commenges organised a session of the French Region at the "Journées de Statistiques" (Avignon),
Robin Genuer Co-organises a reading group called Smiling in Bordeaux
Boris Hejblum organizes the Biostatistics Seminar Series at the Bordeaux Public Health Inserm Research Center
Mélanie Prague organized the "Déjeuners scientifiques" at the "Journées de la statistique française" 2017 and 2018.
Rodolphe Thiébaut organised a summer school course « Statistical analysis of big data in immunology », 14 participants from The Netherlands, Germany, UK and France. All the team members helped in the ground organisation and were involved in teaching. (http://bss-publichealth.u-bordeaux.fr/en/Teaching-team/Course-n-1-Statistical-analysis-of-big-data-linked-to-immunology-systems/r745.html)

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees
Daniel Commenges was a member of the scientific committee of the SFB (French Region of the International Biometric Society) and GdR "Statistique et Santé" conference in Bordeaux (http://gdr-stat-sante.math.cnrs.fr/spip/spip.php?rubrique20),

10.1.2.2. Member of the Conference Program Committees

Daniel Commenges is a member of the scientific committee of the International Biometric Conference Barcelona, July 2018 (http://2018.biometricconference.org).

Mélanie Prague is a member of the scientific committee of CIMI conference “Statistics in Health - personalised medicine” (http://www.cimi.univ-toulouse.fr/mib/en/conference-statistics-and-health), Toulouse 2018, 10-12 January

Mélanie Prague is a member of the scientific committee of the "Déjeuners scientifiques” at the "Journées de la statistique française” 2017 and 2018.

Rodolphe Thiébaut was a member of the scientific committee of the national conference on clinical research (EPICLIN)

Rodolphe Thiébaut was a member of the scientific committee of the IWHOD International Workshop on HIV Observational Databases since 2013 (http://newsite.iwhod.org/Committee)

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

Lifetime Data Analysis (Daniel Commenges)
Statistics Surveys (Daniel Commenges)
2017 IMIA Yearb Med Inform, section editor (Rodolpe Thiébaut)

10.1.3.2. Reviewer - Reviewing Activities

AIDS (Rodolphe Thiébaut)
Annals of Applied Statistics (Boris Hejblum)
Annals of Statistics (Robin Genuer)
Am J Epidemiol (Marta Avalos)
Am J Public Health (Mélanie Prague)
BioData Mining (Boris Hejblum)
Biostatistics (Laura Richert)
Biometrics (Mélanie Prague)
IMIA Yearb Med Inform (Marta Avalos)
International Journal of Epidemiology (Daniel Commenges)
Journal of the Royal Statistical Society: Interaction (Mélanie Prague)
Machine Learning (Robin Genuer)
Neural Information Processing Systems (Robin Genuer)
Pattern Recognition Letters (Robin Genuer)
JRSS-B (Mélanie Prague)
Scientific Reports (Laura Richert)
Society of clinical trial (Mélanie Prague)
Statistical Methods in Medical Research (Robin Genuer, Mélanie Prague)
Statistical science (Mélanie Prague)
Statistics in Medicine (Marta Avalos)

10.1.4. Invited Talks
Rodolpe Thiébaut gave 3 invited talks. He gave an invited talk titled “Objets connectés et Big Data” at the conference “10 ANS DE L’IRESP : Journées de la recherche en santé publique”

Daniel Commenges gave 2 invited talks: Evidence based Medicine (Canterbury) and Biopharmaceutical group of the French Statistical Society (Paris)

Mélanie Prague gave 3 invited talks (Philadelphia Upenn, Boston Harvard school of public health, Inria Bordeaux) and had an invited session in Society for clinical trials, Liverpool, UK (11-14 Mai 2017) on “Integrate approaches for analysis of cluster randomised trials. New development in analysis .”

Robin Genuer was invited to the “Recent advances in tree-based methods (EO380)” session of ERCIM2017, by Ruoqing Zhu (University of Illinois Urbana-Champaign).

Boris Hejblum gave 2 invited talks on Dirichlet process mixtures of multivariate skew t-distributions for unsupervised clustering of cell populations from flow-cytometry data at The Biostatistics Unit at the Cambridge University (UK)

Marta Avalos gave 2 invited talks at the National Centre for Epidemiology & Population Health at the Australian National University, Canberra (Australia), April 2017 and at CSIRO’s Data61, Canberra (Australia), February 2017

Chloé Pasin gave an invited talk at the Probability-Statistics seminar of the Institute Montpellierien Alexander Grothendieck, Montpellier

10.1.5. Leadership within the Scientific Community

Rodolpe Thiébaut and Chloé Pasin are elected members of the ‘collège des écoles doctorales’, University of Bordeaux

Daniel Commenges is President of the French Region of the International Biometric Society

Mélanie Prague is an elected member of the “Young statistician group” of SFdS (French Society of Statistics)

Mélanie Prague and Boris Hejblum are part of the group responsible for the communication of the SFdS - in charge of organising the sponsoring of the society by public and private companies.

Laura Richert is a member of F-CRIN Steering Committee

10.1.6. Scientific Expertise

- Rodolphe Thiébaut is an expert for INCA (Institut National du Cancer) for the PHRC (Programme hospitalier de recherche Clinique en cancérologie) and for the PRME (Programme de recherche médico-économique en cancérologie).
- Rodolphe Thiébaut is a member of the Membre du CNU 46.04 (Biostatistiques, informatique médicale et technologies de communication).
- Rodolphe Thiébaut is a member of the Scientific Council of INSERM.
- Rodolphe Thiébaut is a member of the commitee “Biologie des Systèmes et Cancer (Plan Cancer)”, a member of the Scientific Advisory Board of the “Institut Pierre Louis d’Épidémiologie et de Santé Publique” (UPMC, Dir : Dominique Costagliola), a member of the independent committee of international trials ODYSSEY and SMILE, a member of the scientific council of Muraz’s Center (Bobo-Dioulasso, Burkina Faso).
- Mélanie Prague is an expert for ANRS (France Recherche Nord&Sud Sida-HIV Hépatites) in the CSS 3 (Recherches cliniques et physiopathologiques dans l’infection à VIH).
- Laura Richert is an expert for the PHRC (Programme hospitalier de recherche Clinique).
- Marta Avalos is an expert for L’ASNM (Agence nationale de sécurité du médicament et des produits de santé)

10.1.7. Research Administration
Daniel Commenges is the director of the Biostat-Info axis in the Inserm BPH (Bordeaux Public Health) institute.

Rodolphe Thiébaut is an elected member of the research committee (health sector) in University of Bordeaux and a member of the INSERM Scientific Council

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

In class teaching

Master : Robin Genuer, teaches in the two years of the Master of Public Health (M1 Santé publique, M2 Biostatistique) and 2nd year of the "Modélisation Stochastique et Statistique" Master, University of Bordeaux.

Master : Boris Hejblum, teaches in the two years of the Master of Public Health (M1 Santé publique, M2 Biostatistique).

Master : Rodolphe Thiébaut, teaches in the two years of the Master of Public Health, and he is head of the Epidemiology specialty of the second year of the Master of Public Health.

Master : Laura Richert teaches in the Master of Public Health at ISPED, Univ. Bordeaux, France (M2 Biostatistiques, M2 Épidémiologie).

Master : Mélanie Prague teaches in the Master of Public Health at ISPED, Univ. Bordeaux, France (M2 Biostatistiques).

Master : Marta Avalos teaches in the two years of the Master of Public Health (M1 Santé publique, M2 Biostatistique) at ISPED, Univ. Bordeaux and the 2nd year of the Biostatistics Master, University of Valencia (Spain).

Master : Chloé Pasin, Laura Villain, Hadrien Lorenzo and Louis Capitaine are teaching assistants for the two years.

Edouard Lhomme teaches in the Master of Public Health at ISPED, Univ. Bordeaux (M2 Épidémiologie) and in the Master of Vaccinology from basic immunology to social sciences of health (University Paris-Est Créteil, UPEC)

Bachelor : Laura Richert teaches in PACES and DFASM1-3 for Medical degree at Univ. Bordeaux

Edouard Lhomme teaches in PACES and DFASM1-3 for Medical degree at Univ. Bordeaux

Bachelor : Mélanie Prague and Boris Hejblum teach in the third year ingenious school ENSAI, Rennes.

Summer School: All the SISTM team member teach in the ISPED Summer school.

E-learning

Marta Avalos is head of the first year of the e-learning program of the Master of Public Health, and teaches in it.

Mélanie Prague teaches in the Diplôme universitaire "Méthodes statistiques de régression en épidémiologie".

Boris Hejblum teaches in the Diplôme universitaire "Méthodes statistiques en santé.

Laura Richert teaches in the Diplôme universitaire "Recherche Clinique".

Robin Genuer participated to the IdEx Bordeaux University "Défi numérique" project "BeginR" (http://beginr.moutault.net/).

10.2.2. Supervision

PhD in progress : Chloé Pasin, *Modelling the immune response to HIV vaccine*, from Sep 2015, co-directed by Rodolphe Thiébaut and Francois Dufour.

PhD in progress : Wenjia Wang "Modèle de Rasch", co-directed by Daniel Commenges with Mickael Guedj CIFRE Pharnext, from Oct 2015.

PhD in progress : Laura Villain "Modélisation de l’effet du traitement par injection IL7", co-directed by Daniel Commenges and Rodolphe Thiébaut, from Oct 2015.

PhD in progress : Mélanie Née *Recherche et caractérisation de profils attentionnels : mieux comprendre la place de l’attention dans la survenue des accidents de la vie courante*, from Oct 2015, co-directed by Emmanuel Lagarde, Cédric Galera and Marta Avalos.


Master internship : Louis Capitaine, *Random forests for high dimensional longitudinal data*, directed by Robin Genuer (27/02/2017 - 31/08/2017)

Master internship : Paul Tauzia, *Utilisation de la déconvolution cellulaire pour détecter des différences d’expression génique*, directed by Mélanie Prague and Boris Hejblum (01/03/2017 - 31/08/2017)

Master internship : Augusta Alphonse, *Proof of concept for an automated gating tool applied to flow cytometry data from a HIV therapeutic vaccine trial*, directed by Mélanie Prague and Boris Hejblum (01/07/2017 - 31/07/2017)

Master internship : Marie Alexandre, *Correlation between cellular and antibodies response in Ebola vaccine*, directed by Mélanie Prague (01/06/2017 - 31/08/2017)

10.2.3. Juries

Daniel Commenges was involved in the PhD defences jury of Mr Adjakossa (Paris).

Robin Genuer was a PhD thesis examiner of Wei FENG thesis, defended the 07/19, "Investigation of training data issues in ensemble classification based on margin concept. Application to land cover mapping".

Mélanie Prague is a member of the follow-up dissertation comity of Nicolo Chiara (working on "Mathematical modeling of systemic aspects of cancer and cancer therapy"), Sébastien Benzckery’s PhD student (Inria Bordeaux Sud-ouest, MONC team) and Thiébaut Larivière (working on “Population Kalman estimation in Partial differential equations”), Annabelle Colin’s PhD student (Inria Bordeaux Sud-ouest, MONC team).

Marta Avalos was a member of the follow-up dissertation comity of her PhD students Perrine Soret and Mélanie Née.
Rodolphe Thiébaut took part in the HDR committee of Patricia Thebault, Benoit Lepage, Simon Cauchemez, Sébastien Benzekry and Romulus Breban.

Rodolphe Thiébaut was involved in the PhD defences jury of Nicky De La Mata and Edouard Ollier.

Mélanie Prague took part in the recruitment commission MCF CNU 26 (CNAM).

Laura Richert, Rodolphe Thiébaut, Robin Genuer, Boris Hejblum and Marta Avalos participated to the juries of Master in Public Health (Biostatistics, Epidemiology)

Edouard Lhomme participated to the juries of two medical thesis defense, Medical School of Bordeaux University

10.3. Popularization

Participation to the Inria magazines “Plug-in” and “So news” (Mélanie Prague).

Participation in "The ou café" in Inria Bordeaux (Mélanie Prague).

Lightning talk to present the NIMROD software in Dev Days at Inria (Mélanie Prague).

Edouard Lhomme, as President of AquitHealth, a non profit organisation for the development of e-Health in south west France organized the When Doctors Meet Hackers (WDMH) Congress 2017. The WDMH Congress is a 3 day event with one day of conference on the futur of health and 50 hours of hackathon. The Hackathon is a human adventure where healthcare professionals, patients, developers, designers and entrepreneurs collaborate over a weekend to develop prototypes of eHealth solutions. Six WDMH meetups were also organised each month from January to June 2017 in Bordeaux to discuss about several e-health topics (teledmedecine, data protection, simulation, ...)

11. Bibliography

Major publications by the team in recent years


**Publications of the year**

**Articles in International Peer-Reviewed Journal**


[24] N. Mélanie, M. F. Avalos, A. LUXCEY, B. CONTRAND, L. R. SALMI, A. FOURRIER-REGLAT, B. GADEGBEKU, E. LAGARDE, L. ORRIOLS. Prescription medicine use by pedestrians and the risk of...
injuries road traffic crashes: A case-crossover study, in "PLoS Medicine", 2017, https://hal.inria.fr/hal-01577941.


National Conferences with Proceeding


Conferences without Proceedings


[37] P. SORET, M. F. AVALOS, S. CHENG, R. THIEBAUT. High-dimensional compositional microbiota data: state-of-the-art of methods and software implementations, in "2017 - GDR « Statistiques et santé »", Bordeaux, France, October 2017, https://hal.inria.fr/hal-01667295.

Other Publications


[40] M. PRAGUE, D. COMMENGES, R. THIÉBAUT. In Silico Evaluation of HIV Short-cycle Therapies with Dynamical Models, August 2017, Keystone Symposium, Poster, https://hal.inria.fr/hal-01579070.

References in notes


Project-Team STORM

STatic Optimizations, Runtime Methods

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing
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Project-Team STORM

Creation of the Team: 2015 January 01, updated into Project-Team: 2017 July 01

Keywords:

**Computer Science and Digital Science:**
- A1.1.1. - Multicore, Manycore
- A1.1.2. - Hardware accelerators (GPGPU, FPGA, etc.)
- A1.1.3. - Memory models
- A1.1.4. - High performance computing
- A1.1.5. - Exascale
- A2.2.1. - Static analysis
- A2.2.2. - Memory models
- A2.2.3. - Run-time systems
- A2.2.4. - Parallel architectures
- A2.2.5. - GPGPU, FPGA, etc.

**Other Research Topics and Application Domains:**
- B2.2.1. - Cardiovascular and respiratory diseases
- B3.2. - Climate and meteorology
- B3.3.1. - Earth and subsoil
- B3.4.1. - Natural risks
- B4.2. - Nuclear Energy Production
- B5.2.3. - Aviation
- B5.2.4. - Aerospace
- B6.2.2. - Radio technology
- B6.2.3. - Satellite technology
- B6.2.4. - Optic technology

1. Personnel

**Research Scientists**
- Olivier Aumage [Inria, Researcher]
- Emmanuelle Saillard [Inria, Researcher, from Oct 2017]

**Faculty Members**
- Denis Barthou [Team leader, Institut National Polytechnique de Bordeaux, Professor, HDR]
- Marie-Christine Counilh [Univ de Bordeaux, Associate Professor]
- Raymond Namyst [Univ de Bordeaux, Professor, HDR]
- Samuel Thibault [Univ de Bordeaux, Associate Professor]
- Pierre-André Wacrenier [Univ de Bordeaux, Associate Professor]

**External Collaborators**
- Adrien Cassagne [Institut National Polytechnique de Bordeaux, until Sep 2017]
- Terry Cojean [Univ de Bordeaux, from Sep 2017]

**Technical Staff**
- Jérôme Clet-Ortega [Inria, until Feb 2017]
2. Overall Objectives

2.1. Overall Objectives

A successful approach to deal with the complexity of modern architectures is centered around the use of runtime systems, to manage tasks dynamically, these runtime systems being either generic or specific to an application. Similarly, on the compiler side, optimizations and analyses are more aggressive in iterative compilation frameworks, fit for library generations, or DSL, in particular for linear algebra methods. To go beyond this state of the art and alleviate the difficulties for programming these machines, we believe it is necessary to provide inputs with richer semantics to runtime and compiler alike, and in particular by combining both approaches.

This general objective is declined into two sub-objectives, the first concerning the expression of parallelism itself, the second the optimization and adaptation of this parallelism by compilers and runtimes.

- Expressing parallelism: As shown in the following figure, we propose to work on parallelism expression through Domain Specific Languages, able to capture the essence of the algorithms used through usual parallel languages such as OpenCL, OpenMP and through high performance libraries. The DSLs will be driven by applications, with the idea to capture at the algorithmic level the parallelism of the problem and perform dynamic data layout adaptation, parallel and algorithmic optimizations. The principle here is to capture a higher level of semantics, enabling users to express not only parallelism but also different algorithms.

- Optimizing and adapting parallelism: The goal here is to leverage the necessary adaptation to evolving hardware, by providing mechanisms allowing users to run the same code on different architectures. This implies to adapt parallelism, in particular the granularity of the work, to the architecture. This relies on the use of existing parallel libraries and their composition, and more generally the separation of concern between the description of tasks, that represent semantic units of work, and the tasks to be executed by the different processing units. Splitting or coarsening moldable tasks, generating code for these tasks and scheduling them is part of this work.
Figure 1. STORM Big Picture
Finally, the abstraction we advocate for requires to propose a feedback loop. This feedback has two objectives: To make users better understand their application and how to change the expression of parallelism if necessary, but also to propose an abstracted model for the machine. This allows to develop and formalize the compiling, scheduling techniques on a model, not too far from the real machine. Here, simulation techniques are a way to abstract the complexity of the architecture while preserving essential metrics.

3. Research Program

3.1. Parallel Computing and Architectures

Following the current trends of the evolution of HPC systems architectures, it is expected that future Exascale systems (i.e. Sustaining $10^{18}$ flops) will have millions of cores. Although the exact architectural details and trade-offs of such systems are still unclear, it is anticipated that an overall concurrency level of $O(10^9)$ threads/tasks will probably be required to feed all computing units while hiding memory latencies. It will obviously be a challenge for many applications to scale to that level, making the underlying system sound like “embarrassingly parallel hardware.”

From the programming point of view, it becomes a matter of being able to expose extreme parallelism within applications to feed the underlying computing units. However, this increase in the number of cores also comes with architectural constraints that actual hardware evolution prefigures: computing units will feature extra-wide SIMD and SIMT units that will require aggressive code vectorization or “SIMDization”, systems will become hybrid by mixing traditional CPUs and accelerators units, possibly on the same chip as the AMD APU solution, the amount of memory per computing unit is constantly decreasing, new levels of memory will appear, with explicit or implicit consistency management, etc. As a result, upcoming extreme-scale system will not only require unprecedented amount of parallelism to be efficiently exploited, but they will also require that applications generate adaptive parallelism capable to map tasks over heterogeneous computing units.

The current situation is already alarming, since European HPC end-users are forced to invest in a difficult and time-consuming process of tuning and optimizing their applications to reach most of current supercomputers’ performance. It will go even worse at horizon 2020 with the emergence of new parallel architectures (tightly integrated accelerators and cores, high vectorization capabilities, etc.) featuring unprecedented degree of parallelism that only too few experts will be able to exploit efficiently. As highlighted by the ETP4HPC initiative, existing programming models and tools won’t be able to cope with such a level of heterogeneity, complexity and number of computing units, which may prevent many new application opportunities and new science advances to emerge.

The same conclusion arises from a non-HPC perspective, for single node embedded parallel architectures, combining heterogeneous multicores, such as the ARM big.LITTLE processor and accelerators such as GPUs or DSPs. The need and difficulty to write programs able to run on various parallel heterogeneous architectures has led to initiatives such as HSA, focusing on making it easier to program heterogeneous computing devices. The growing complexity of hardware is a limiting factor to the emergence of new usages relying on new technology.

3.2. Scientific and Societal Stakes

In the HPC context, simulation is already considered as a third pillar of science with experiments and theory. Additional computing power means more scientific results, and the possibility to open new fields of simulation requiring more performance, such as multi-scale, multi-physics simulations. Many scientific domains able to take advantage of Exascale computers, these “Grand Challenges” cover large panels of science, from seismic, climate, molecular dynamics, theoretical and astrophysics physics... Besides, embedded applications are also able to take advantage of these performance increase. There is still an on-going trend where dedicated hardware is progressively replaced by off-the-shelf components, adding more adaptability and lowering the cost of
devices. For instance, Error Correcting Codes in cell phones are still hardware chips, but with the forthcoming 5G protocol, new software and adaptative solutions relying on low power multicore are also explored. New usages are also appearing, relying on the fact that large computing capacities are becoming more affordable and widespread. This is the case for instance with Deep Neural Networks where the training phase can be done on supercomputers and then used in embedded mobile systems. The same consideration applies for big data problems, of internet of things, where small sensors provide large amount of data that need to be processed in short amount of time. Even though the computing capacities required for such applications are in general a different scale from HPC infrastructures, there is still a need in the future for high performance computing applications.

However, the outcome of new scientific results and the development of new usages for mobile, embedded systems will be hindered by the complexity and high level of expertise required to tap the performance offered by future parallel heterogeneous architectures.

3.3. Towards More Abstraction

As emphasized by initiatives such as the European Exascale Software Initiative (EESI), the European Technology Platform for High Performance Computing (ETP4HPC), or the International Exascale Software Initiative (IESP), the HPC community needs new programming APIs and languages for expressing heterogeneous massive parallelism in a way that provides an abstraction of the system architecture and promotes high performance and efficiency. The same conclusion holds for mobile, embedded applications that require performance on heterogeneous systems.

This crucial challenge given by the evolution of parallel architectures therefore comes from this need to make high performance accessible to the largest number of developers, abstracting away architectural details providing some kind of performance portability. Disruptive uses of the new technology and groundbreaking new scientific results will not come from code optimization or task scheduling, but they require the design of new algorithms that require the technology to be tamed in order to reach unprecedented levels of performance.

Runtime systems and numerical libraries are part of the answer, since they may be seen as building blocks optimized by experts and used as-is by application developers. The first purpose of runtime systems is indeed to provide abstraction. Runtime systems offer a uniform programming interface for a specific subset of hardware (e.g., OpenGL or DirectX are well-established examples of runtime systems dedicated to hardware-accelerated graphics) or low-level software entities (e.g., POSIX-thread implementations). They are designed as thin user-level software layers that complement the basic, general purpose functions provided by the operating system calls. Applications then target these uniform programming interfaces in a portable manner. Low-level, hardware dependent details are hidden inside runtime systems. The adaptation of runtime systems is commonly handled through drivers. The abstraction provided by runtime systems thus enables portability. Abstraction alone is however not enough to provide portability of performance, as it does nothing to leverage low-level-specific features to get increased performance. Consequently, the second role of runtime systems is to optimize abstract application requests by dynamically mapping them onto low-level requests and resources as efficiently as possible. This mapping process makes use of scheduling algorithms and heuristics to decide the best actions to take for a given metric and the application state at a given point in its execution time. Thus, optimization together with abstraction allows runtime systems to offer portability of performance. Numerical libraries provide sets of highly optimized kernels for a given field (dense or sparse linear algebra, FFT, etc.) either in an autonomous fashion or using an underlying runtime system.

Application domains cannot resort to libraries for all codes however, computation patterns such as stencils are a representative example of such difficulty. The compiler technology plays here a central role, in managing high level semantics, either through templates, domain specific languages or annotations. Compiler optimizations, and the same applies for runtime optimizations, are limited by the level of semantics they manage. Providing part of the algorithmic knowledge of an application, for instance knowing that it computes a 5-point stencil and then performs a dot product, would lead to more opportunities to adapt parallelism, memory structures, and is a way to leverage the evolving hardware.
Compilers and runtime play a crucial role in the future of high performance applications, by defining the input language for users, and optimizing/transforming it into high performance code. The objective of STORM is to propose better interactions between compiler and runtime and more semantics for both approaches. We recall in the following section the expertise of the team.

4. Application Domains

4.1. Application Domains

The application of our work concerns linear algebra, solvers and fast-multipole methods, in collaboration with other Inria teams and with industry. This allows a wide range of scientific and industrial applications possibly interested in the techniques we propose, in the domain of high performance computing but also in order to compute intensive embedded applications. In terms of direct application, the software developed in the team are used in applications in various fields, ranging from seismic, mechanic of fluids, molecular dynamics, high energy physics or material simulations. Similarly, the domains of image processing and signal processing can take advantage of the expertise and software of the team.

5. New Software and Platforms

5.1. Chameleon

**KEYWORDS:** Runtime system - Task-based algorithm - Dense linear algebra - HPC - Task scheduling

**SCIENTIFIC DESCRIPTION:** Chameleon is part of the MORSE (Matrices Over Runtime Systems @ Exascale) project. The overall objective is to develop robust linear algebra libraries relying on innovative runtime systems that can fully benefit from the potential of those future large-scale complex machines.

We expect advances in three directions based first on strong and closed interactions between the runtime and numerical linear algebra communities. This initial activity will then naturally expand to more focused but still joint research in both fields.

1. Fine interaction between linear algebra and runtime systems. On parallel machines, HPC applications need to take care of data movement and consistency, which can be either explicitly managed at the level of the application itself or delegated to a runtime system. We adopt the latter approach in order to better keep up with hardware trends whose complexity is growing exponentially. One major task in this project is to define a proper interface between HPC applications and runtime systems in order to maximize productivity and expressivity. As mentioned in the next section, a widely used approach consists in abstracting the application as a DAG that the runtime system is in charge of scheduling. Scheduling such a DAG over a set of heterogeneous processing units introduces a lot of new challenges, such as predicting accurately the execution time of each type of task over each kind of unit, minimizing data transfers between memory banks, performing data prefetching, etc. Expected advances: In a nutshell, a new runtime system API will be designed to allow applications to provide scheduling hints to the runtime system and to get real-time feedback about the consequences of scheduling decisions.

2. Runtime systems. A runtime environment is an intermediate layer between the system and the application. It provides low-level functionality not provided by the system (such as scheduling or management of the heterogeneity) and high-level features (such as performance portability). In the framework of this proposal, we will work on the scalability of runtime environment. To achieve scalability it is required to avoid all centralization. Here, the main problem is the scheduling of the tasks. In many task-based runtime environments the scheduler is centralized and becomes a bottleneck as soon as too many cores are involved. It is therefore required to distribute the scheduling decision or to compute a data distribution that impose the mapping of task using, for instance the so-called “owner-compute” rule. Expected advances: We will design runtime systems that enable an efficient and scalable use of thousands of distributed multicore nodes enhanced with accelerators.
3. Linear algebra. Because of its central position in HPC and of the well understood structure of its algorithms, dense linear algebra has often pioneered new challenges that HPC had to face. Again, dense linear algebra has been in the vanguard of the new era of petascale computing with the design of new algorithms that can efficiently run on a multicore node with GPU accelerators. These algorithms are called “communication-avoiding” since they have been redesigned to limit the amount of communication between processing units (and between the different levels of memory hierarchy). They are expressed through Direct Acyclic Graphs (DAG) of fine-grained tasks that are dynamically scheduled. Expected advances: First, we plan to investigate the impact of these principles in the case of sparse applications (whose algorithms are slightly more complicated but often rely on dense kernels). Furthermore, both in the dense and sparse cases, the scalability on thousands of nodes is still limited, new numerical approaches need to be found. We will specifically design sparse hybrid direct/iterative methods that represent a promising approach.

Overall end point. The overall goal of the MORSE associate team is to enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

**FUNCTIONAL DESCRIPTION:** Chameleon is a dense linear algebra software relying on sequential task-based algorithms where sub-tasks of the overall algorithms are submitted to a Runtime system. A Runtime system such as StarPU is able to manage automatically data transfers between not shared memory area (CPUs-GPUs, distributed nodes). This kind of implementation paradigm allows to design high performing linear algebra algorithms on very different type of architecture: laptop, many-core nodes, CPUs-GPUs, multiple nodes. For example, Chameleon is able to perform a Cholesky factorization (double-precision) at 80 TFlop/s on a dense matrix of order 400 000 (e.i. 4 min).

**RELEASE FUNCTIONAL DESCRIPTION:** Chameleon includes the following features:
- BLAS 3, LAPACK one-sided and LAPACK norms tile algorithms
- Support QUARK and StarPU runtime systems
- Exploitation of homogeneous and heterogeneous platforms through the use of BLAS/LAPACK CPU kernels and cuBLAS/MAGMA CUDA kernels
- Exploitation of clusters of interconnected nodes with distributed memory (using OpenMPI)

**Participants:** Cédric Castagnoedd, Samuel Thibault, Emmanuel Agullo, Florent Pruvost and Mathieu Faverge

**Partners:** Innovative Computing Laboratory (ICL) - King Abdullha University of Science and Technology - University of Colorado Denver

**Contact:** Emmanuel Agullo

**URL:** [https://project.inria.fr/chameleon/](https://project.inria.fr/chameleon/)

5.2. hwloc

**Hardware Locality**

**KEYWORDS:** NUMA - Multicore - GPU - Affinities - Open MPI - Topology - HPC - Locality

**FUNCTIONAL DESCRIPTION:** Hardware Locality (hwloc) is a library and set of tools aiming at discovering and exposing the topology of machines, including processors, cores, threads, shared caches, NUMA memory nodes and I/O devices. It builds a widely-portable abstraction of these resources and exposes it to applications so as to help them adapt their behavior to the hardware characteristics. They may consult the hierarchy of resources, their attributes, and bind task or memory on them.

hwloc targets many types of high-performance computing applications, from thread scheduling to placement of MPI processes. Most existing MPI implementations, several resource managers and task schedulers, and multiple other parallel libraries already use hwloc.

**Participants:** Brice Goglin and Samuel Thibault

**Partners:** Open MPI consortium - Intel - AMD

**Contact:** Brice Goglin
• Publications: hwloc: a Generic Framework for Managing Hardware Affinities in HPC Applications
  - Managing the Topology of Heterogeneous Cluster Nodes with Hardware Locality (hwloc) - A Topology-Aware Performance Monitoring Tool for Shared Resource Management in Multicore Systems - Exposing the Locality of Heterogeneous Memory Architectures to HPC Applications - Towards the Structural Modeling of the Topology of next-generation heterogeneous cluster Nodes with hwloc - On the Overhead of Topology Discovery for Locality-aware Scheduling in HPC
  • URL: http://www.open-mpi.org/projects/hwloc/

5.3. KaStORS

The KaStORS OpenMP Benchmark Suite

KEYWORDS: OpenMP - Task scheduling - Task-based algorithm - HPC - Benchmarking - Data parallelism
FUNCTIONAL DESCRIPTION: The KaStORS benchmarks suite has been designed to evaluate implementations of the OpenMP dependent task paradigm, introduced as part of the OpenMP 4.0 specification.
  • Participants: François Broquedis, Nathalie Furmento, Olivier Aumage, Philippe Virouleau, Pierrick Brunet, Samuel Thibault and Thierry Gautier
  • Contact: Thierry Gautier
  • URL: http://kastors.gforge.inria.fr/#!index.md

5.4. KStar

The KStar OpenMP Compiler

KEYWORDS: Source-to-source compiler - OpenMP - Task scheduling - Compilers - Data parallelism
FUNCTIONAL DESCRIPTION: The KStar software is a source-to-source OpenMP compiler for languages C and C++. The KStar compiler translates OpenMP directives and constructs into API calls from the StarPU runtime system or the XKaapi runtime system. The KStar compiler is virtually fully compliant with OpenMP 3.0 constructs. The KStar compiler supports OpenMP 4.0 dependent tasks and accelerated targets.
  • Participants: Nathalie Furmento, Olivier Aumage, Samuel Pitoiset and Samuel Thibault
  • Contact: Olivier Aumage
  • URL: http://kstar.gforge.inria.fr/#!index.md

5.5. MAQAO

SCIENTIFIC DESCRIPTION: MAQAO relies on binary codes for Intel x86 and ARM architectures. For x86 architecture, it can insert probes for instrumentation directly inside the binary. There is no need to recompile. The static/dynamic approach of MAQAO analysis is the main originality of the tool, combining performance model with values collected through instrumentation.

MAQAO has a static performance model for x86 and ARM architectures. This model analyzes performance of the codes on the architectures and provides some feed-back hints on how to improve these codes, in particular for vector instructions.

The dynamic collection of data in MAQAO enables the analysis of thread interactions, such as false sharing, amount of data reuse, runtime scheduling policy, ...

FUNCTIONAL DESCRIPTION: MAQAO is a performance tuning tool for OpenMP parallel applications. It relies on the static analysis of binary codes and the collection of dynamic information (such as memory traces). It provides hints to the user about performance bottlenecks and possible workarounds.
  • Participants: Christopher Haine, Denis Barthou, James Tombi A Mba and Olivier Aumage
  • Contact: Denis Barthou

5.6. StarPU

The StarPU Runtime System
**KEYWORDS:** Multicore - GPU - Scheduling - HPC - Performance

**SCIENTIFIC DESCRIPTION:** Traditional processors have reached architectural limits which heterogeneous multicore designs and hardware specialization (e.g. coprocessors, accelerators, ...) intend to address. However, exploiting such machines introduces numerous challenging issues at all levels, ranging from programming models and compilers to the design of scalable hardware solutions. The design of efficient runtime systems for these architectures is a critical issue. StarPU typically makes it much easier for high performance libraries or compiler environments to exploit heterogeneous multicore machines possibly equipped with GPGPUs or Cell processors: rather than handling low-level issues, programmers may concentrate on algorithmic concerns. Portability is obtained by the means of a unified abstraction of the machine. StarPU offers a unified offloadable task abstraction named "codelet". Rather than rewriting the entire code, programmers can encapsulate existing functions within codelets. In case a codelet may run on heterogeneous architectures, it is possible to specify one function for each architecture (e.g. one function for CUDA and one function for CPUs).

StarPU takes care to schedule and execute those codelets as efficiently as possible over the entire machine. In order to relieve programmers from the burden of explicit data transfers, a high-level data management library enforces memory coherency over the machine: before a codelet starts (e.g. on an accelerator), all its data are transparently made available on the compute resource. Given its expressive interface and portable scheduling policies, StarPU obtains portable performances by efficiently (and easily) using all computing resources at the same time. StarPU also takes advantage of the heterogeneous nature of a machine, for instance by using scheduling strategies based on auto-tuned performance models.

StarPU is a task programming library for hybrid architectures

The application provides algorithms and constraints: - CPU/GPU implementations of tasks - A graph of tasks, using either the StarPU’s high level GCC plugin pragmas or StarPU’s rich C API

StarPU handles run-time concerns - Task dependencies - Optimized heterogeneous scheduling - Optimized data transfers and replication between main memory and discrete memories - Optimized cluster communications

Rather than handling low-level scheduling and optimizing issues, programmers can concentrate on algorithmic concerns!

**FUNCTIONAL DESCRIPTION:** StarPU is a runtime system that offers support for heterogeneous multicore machines. While many efforts are devoted to design efficient computation kernels for those architectures (e.g. to implement BLAS kernels on GPUs), StarPU not only takes care of offloading such kernels (and implementing data coherency across the machine), but it also makes sure the kernels are executed as efficiently as possible.

- Participants: Corentin Salingue, Andra Hugo, Benoît Lize, Cédric Augonnet, Cyril Roelandt, François Tessier, Jérôme Clet-Ortega, Ludovic Courtes, Ludovic Stordeur, Marc Sergent, Mehdi Juhoor, Nathalie Furmento, Nicolas Collin, Olivier Aumage, Pierre-André Wacrenier, Raymond Namyst, Samuel Thibault, Simon Archipoff and Xavier Lacoste

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### 5.7. PARCOACH

**PARallel Control flow Anomaly CHecker**

**KEYWORDS:** High-Performance Computing - Program verification - Debug - MPI - OpenMP - Compilation

**SCIENTIFIC DESCRIPTION:** PARCOACH verifies programs in two steps. First, it statically verifies applications with a data- and control-flow analysis and outlines execution paths leading to potential deadlocks. The code is then instrumented, displaying an error and synchronously interrupting all processes if the actual scheduling leads to a deadlock situation.
**FUNCTIONAL DESCRIPTION**: Supercomputing plays an important role in several innovative fields, speeding up prototyping or validating scientific theories. However, supercomputers are evolving rapidly with now millions of processing units, posing the questions of their programmability. Despite the emergence of more widespread and functional parallel programming models, developing correct and effective parallel applications still remains a complex task. As current scientific applications mainly rely on the Message Passing Interface (MPI) parallel programming model, new hardwares designed for Exascale with higher node-level parallelism clearly advocate for an MPI+X solutions with X a thread-based model such as OpenMP. But integrating two different programming models inside the same application can be error-prone leading to complex bugs - mostly detected unfortunately at runtime. PARallel COntrol flow Anomaly CHecker aims at helping developers in their debugging phase.

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- **URL**: https://esaillar.github.io/PARCOACH/

### 5.8. AFF3CT

**A Fast Forward Error Correction Tool**

**KEYWORDS**: High-Performance Computing - Signal processing - Error Correction Code

**FUNCTIONAL DESCRIPTION**: AFF3CT proposes high performance Error Correction algorithms for Polar, Turbo, LDPC, RSC (Recursive Systematic Convolutional), Repetition and RA (Repeat and Accumulate) codes. These signal processing codes can be parameterized in order to optimize some given metrics, such as Bit Error Rate, Bandwidth, Latency, ...using simulation. For the designers of such signal processing chain, AFF3CT proposes also high performance building blocks so to develop new algorithms. AFF3CT compiles with many compilers and runs on Windows, Mac OS X, Linux environments and has been optimized for x86 (SSE, AVX instruction sets) and ARM architectures (NEON instruction set).

- **Authors**: Adrien Cassagne, Bertrand Le Gal, Camille Leroux, Denis Barthou and Olivier Aumage
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- **URL**: https://aff3ct.github.io/

### 5.9. MORSE

**KEYWORDS**: High performance computing - Matrix calculation - Fast multipole method - Runtime system

**FUNCTIONAL DESCRIPTION**: MORSE (Matrices Over Runtime Systems @ Exascale) is a scientific project, its objectives are to solve matrix problems on complex architectures, using runtime systems. More specifically, the goal is to write codes that reach a high level of performance for all architectures. The algorithms are written independently of the architecture, and the runtime system dispatches the different computational parts to the different computing units. This methodology has been validated on three classes of problems: dense linear algebra, sparse and dense, and fast multipole methods. The corresponding codes have been incorporated into several softwares, MAGMA, Pastix and ScalFMM.

- **Contact**: Emmanuel Agullo
- **URL**: http://icl.cs.utk.edu/morse/
6. New Results

6.1. Distributed Sequential Task Flow with StarPU

The emergence of accelerators as standard computing resources on supercomputers and the subsequent architectural complexity increase revived the need for high-level parallel programming paradigms. Sequential task-based programming model has been shown to efficiently meet this challenge on a single multicore node possibly enhanced with accelerators, which motivated its support in the OpenMP 4.0 standard. We showed [5] that this paradigm can also be employed to achieve high performance on modern supercomputers composed of multiple such nodes, with extremely limited changes in the user code. To prove this claim, we have extended the StarPU runtime system with an advanced inter-node data management layer that supports this model by posting communications automatically. We illustrates our discussion with the task-based tile Cholesky algorithm that we implemented on top of this new runtime system layer. We showed that it enables very high productivity while achieving a performance competitive with both the pure Message Passing Interface (MPI)-based ScalAPACK Cholesky reference implementation and the DPLASMA Cholesky code, which implements another (non-sequential) task-based programming paradigm.

6.2. Distributed StarPU on top of a High Performance Communication Library

A new implementation of the StarPU’s distributed engine is being currently developed on top of the NewMadeleine library. The first version of this engine had been written directly on top of MPI. The performance were not as good as expected when dealing with applications exchanging huge number of messages, and we had to implement within StarPU mechanisms to control the memory subscription [14].

NewMadeleine is a high performance communication library for clusters developed in the Tadaam team. It applies optimization strategy on data flows through dynamic packet scheduling, and is usable on various high performance networks. The new implementation of the StarPU’s distributed engine no longer has to deal with communication-related issues, and provides a better reactivity as the communications progress is dealt with by NewMadeleine itself. First experiments with the Chameleon solver show promising results.

6.3. Bridging the Gap between a Standard Parallel Language and a Task-based Runtime System

With the advent of complex modern architectures, the low-level paradigms long considered sufficient to build High Performance Computing (HPC) numerical codes have met their limits. Achieving efficiency, ensuring portability, while preserving programming tractability on such hardware prompted the HPC community to design new, higher level paradigms while relying on runtime systems to maintain performance. However, the common weakness of these projects is to deeply tie applications to specific expert-only runtime system APIs. The OpenMP specification, which aims at providing common parallel programming means for shared-memory platforms, appears as a good candidate to address this issue thanks to the latest task-based constructs introduced in its revision 4.0. We assessed [4] the effectiveness and limits of this support for designing a high-performance numerical library, ScalFMM, implementing the fast multipole method (FMM) that we have deeply re-designed with respect to the most advanced features provided by OpenMP 4. We showed that OpenMP 4 allows for significant performance improvements over previous OpenMP revisions on recent multicore processors and that extensions to the 4.0 standard allow for strongly improving the performance, bridging the gap with the very high performance that was so far reserved to expert-only runtime system APIs. Our proposal for an OpenMP extension to let the programmer express the property of commutativity between multiple tasks has been presented by Inria and successfully voted-on and integrated as the notion of mutually exclusive input/output sets (mutexinoutset keyword) in OpenMP ARB’s Technical Report 6: OpenMP Version 5.0 Preview 2, the last pre-version of the upcoming OpenMP 5.0 specification.
6.4. Combining a Component Model and a Task Parallelism Model

We demonstrated the feasibility of efficiently combining both a software component model and a task-based model [6]. Task-based models are known to enable efficient executions on recent HPC computing nodes while component models ease the separation of concerns of application and thus improve their modularity and adaptability.

This paper describes a prototype version of the COMET programming model combining concepts of task-based and component models, and a preliminary version of the COMET runtime built on top of StarPU and L2C. Evaluations of the approach have been conducted on a real-world use-case analysis of a sub-part of the production application GYSELA.

Results show that the approach is feasible and that it enables easy composition of independent software codes without introducing overheads. Performance results are equivalent to those obtained with a plain OpenMP based implementation.

6.5. Tackling the granularity problem

One of the main issues encountered when trying to exploit both CPUs and accelerators is that these devices have very different characteristics and requirements. Indeed, GPUs typically exhibit better performance when executing kernels applied to large data sets while regular CPU cores reach their peak performance with fine grain kernels working on a reduced memory footprint. To work around this granularity problem, task-based applications running on such heterogeneous platforms typically adopt a medium granularity, chosen as a trade-off between coarse-grain and fine-grain kernels. To tackle this granularity problem, we investigated different complementary techniques. The first two techniques are based on StarPU, performing both load-balancing and scheduling, the third one splits automatically kernels at compile-time and then performs load-balancing.

- The first technique is based on resource aggregation: we aggregate CPU cores to execute coarse grain tasks in a parallel manner. We have showed that this technique for a dense Cholesky factorization kernel outperforms state of the art implementations on a platform equipped with 24 CPU cores and 4 GPU devices (reaching a peak performance of 4.8 TFlop/s) and on the Intel KNL processor (reaching a peak performance 1.58 TFlop/s).

- The second technique splits dynamically coarse grain tasks when they are assigned to CPU cores. Tasks can be replaced by a subgraph of tasks of finer granularity, allowing for a finer handling of dependencies and a better pipelining of kernels. This mechanism allowing to deal with hierarchical task graphs has been designed within StarPU. Moreover, it allows to parallelize the task submission flow while preserving the simplicity of the sequential task flow submission paradigm. First experimental results for dense Cholesky factorization kernel show good performance improvements with respect to the native StarPU’s implementation.

- The third technique extends our previous work that provides an automatic compiler and runtime technique to execute single OpenCL kernels on heterogeneous multi-device architectures. Our technique splits computation and data automatically across the multiple computing devices. OpenCL applications that consist in a chain of data-dependent kernels in an iterative computation are now considered. The technique proposed is completely transparent to the user, and does not require off-line training or a performance model. It manages sometimes conflicting needs between load balancing each kernel in the chain and minimizing data transfer between consecutive kernels, taking data locality into account. Load-balancing issues, resulting from hardware heterogeneity, load imbalance within a kernel itself, and load variations between repeated executions are also managed.

Experiments on some benchmarks show the interest of our approach and we are currently implementing it in an OpenCL N-body computation with short-range interactions.
6.6. Interfacing MAQAO and BOAST Frameworks for Kernel Autotuning on ARM Platforms

In Project MontBlanc 2’s deliverable D5.11 [13] we presented the integration of STORM’s MAQAO software (a binary-level code analysis framework) with BOAST (an automatic performance tuning framework for metaprogramming and optimizing computing kernels) developed at LIG’s NANOSIM. From source meta-kernels written in the RUBY language, BOAST generates multiple versions, in various target languages, optionally applying optimization transformations and strategies, and exploring the space of compiler flags combinations, to discover the most effective kernel tuning parameters. MAQAO offers a scriptable framework to disassemble kernel binaries, explore binary instruction flows, register-level data dependencies, program control structures, to patch, re-assemble and instrument kernel binaries for tracing data access patterns, and to process them from custom analyzers written in the LUA language. This integration work built on the complementarity of these two environments by enabling MAQAO to process binary kernels generated by BOAST, and lead developers in a guided tuning cycle.

6.7. Using heterogeneous memories

Heterogeneous memories, such as the MCDRAM in the Xeon Phi architecture, with different latency and bandwidth characteristics, complicate the way the users allocate and use memory. In 2017, we have designed, in collaboration with CEA, an automatic tool to characterize the bandwidth needs of an application, in particular finding the functions and the arrays in these functions that would benefit the most of a high bandwidth. This tool is a plugin of gcc, and has been applied successfully to large CORAL benchmarks (Lulesh, MiniFE, AMG2013, Mcb and Snap). This characterization is essential in the common case where all data cannot fit into the MCDRAM but a more selective use of the MCDRAM is needed. The transformation of the memory allocations is automatic, based on these metrics. The development of better metrics, allowing to choose the most appropriate array is on going work.

6.8. Rewriting System for Profile-Guided Data Layout Transformations on Binaries

Careful data layout design is crucial for achieving high performance. However exploring data layouts is time-consuming and error-prone, and assessing the impact of a layout transformation on performance is difficult without performing it. We proposed [7] a method and implemented a prototype to guide application programmers through data layout restructuring for improving kernel performance and SIMDizability, by providing a comprehensive multidimensional description of the initial layout, built from trace analysis, and then by giving a performance evaluation of the transformations tested and an expression of each transformed layout. The programmer can limit the exploration to layouts matching some patterns. We apply this method to two multithreaded applications. The performance prediction of multiple transformations matches within 5% the performance of hand-transformed layout code.

6.9. Correctness of HPC Applications

The current supercomputer hardware trends lead to more complex HPC applications (heterogeneity in hardware and combinations of parallel programming models) that pose programmability challenges. Furthermore, progress to exascale stresses the requirement for convenient and scalable debugging methods to help developers fully exploit the future machines. Despite advances in the domain, this still remains a manual complex task. We aim to develop tools and methods to aid developers with problems of correctness in HPC applications for exascale systems. There are several requirements for such tools: 1) precision - report and handle only real problems, areas of interest; 2) scalability in LoCs and execution time; 3) heterogeneity - ability to handle multiple languages, runtime and execution models; and 4) soundness - ability to prove code properties. In order to improve developer productivity, we aim to develop a combination of static and dynamic analyses. Static analysis techniques will enable soundness and scalability in execution time. Dynamic analysis techniques will enable precision, scalability in LoCs and heterogeneity for hybrid parallelism.
The achieved results this year allow to perform an interprocedural static data- and control-flow analysis: its improves precision, by only detecting possible correctness issues related to MPI rank dependent variables. It improves scalability also by reducing the amount of dead-lock avoiding code added. This new method has been applied to CUDA, MPI, OpenMP and UPC parallel codes to detect collective deadlocks.

6.10. AMR-Based Dynamic Load Balancing for Molecular Dynamics Simulations

Modern parallel architectures require applications to generate enough parallelism to feed many cores, which require in turn regular data-parallel instructions to exploit large vector units. We revisit the extensively-studied Classical Molecular Dynamics N-body problem in the light of these hardware constraints. A new data layout is proposed with efficient force computation methods focusing on adaptive mesh refinement techniques, multi-threading, vectorization-friendly, using low memory footprint. Our design is guided by the need for load balancing and adaptivity raised by highly dynamic particle sets, as typically observed in simulations of strong shocks resulting in material micro-jetting. We analyze performance results on several simulation scenarios, over clusters equipped with Intel Xeon Phi knl processors. Performance obtained with our implementation using OpenMP is close to state-of-the-art implementations (LAMMPS) using MPI on steady particles simulations, and outperform them by 1.2 on micro-jetting simulations on Intel Xeon Phi (KNL).


With the advent of multicore and manycore processors as building blocks of HPC supercomputers, many applications shift from relying solely on a distributed programming model (e.g., MPI) to mixing distributed and shared-memory models (e.g., MPI+OpenMP), to better exploit shared-memory communications and reduce the overall memory footprint. One side effect of this programming approach is runtime stacking: mixing multiple models involve various runtime libraries to be alive at the same time and to share the underlying computing resources. This paper explores different configurations where this stacking may appear and introduces algorithms to detect the misuse of compute resources when running a hybrid parallel application. We have implemented our algorithms inside a dynamic tool that monitors applications and outputs resource usage to the user. We validated this tool on applications from CORAL benchmarks. This leads to relevant information which can be used to improve runtime placement, and to an average overhead lower than 1% of total execution time.

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry


8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. PIA

ELCI  The ELCI project (Software Environment for HPC) aims to develop a new generation of software stack for supercomputers, numerical solvers, runtime and programming development environments for HPC simulation. The ELCI project also aims to validate this software stack by showing its capacity to offer improved scalability, resilience, security, modularity and abstraction on real applications. The coordinator is Bull, and the different partners are CEA, Inria, SAFRAN, CERFACS, CNRS CORIA, CENAERO, ONERA, UVSQ, Kitware and AlgoTech.
8.1.2. ANR

ANR SOLHAR  (http://solhar.gforge.inria.fr/doku.php?id=start).
ANR MONU 2013 Program, 2013 - 2017 (36 months extended )
Identification: ANR-13-MONU-0007
Coordinator: Inria Bordeaux/LaBRI
Other partners: CNRS-IRIT, Inria-LIP Lyon, CEA/CESTA, EADS-IW
Abstract: This project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computers equipped with accelerators. The ultimate aim of this project is to achieve the implementation of a software package providing a solver based on direct methods for sparse linear systems of equations. Several attempts have been made to accomplish the porting of these methods on such architectures; the proposed approaches are mostly based on a simple offloading of some computational tasks (the coarsest grained ones) to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool developed in the runtime team (Bordeaux). Although the SOLHAR project will focus on heterogeneous computers equipped with GPUs due to their wide availability and affordable cost, the research accomplished on algorithms, methods and programming models will be readily applicable to other accelerator devices such as ClearSpeed boards or Cell processors.

ANR Songs Simulation of next generation systems (http://infra-songs.gforge.inria.fr/).
ANR INFRA 2011, 01/2012 - 12/2015 (48 months)
Identification: ANR-11INFR01306
Coordinator: Martin Quinson (Inria Nancy)
Other partners: Inria Nancy, Inria Rhône-Alpes, IN2P3, LSIIT, Inria Rennes, I3S.
Abstract: The goal of the SONGS project is to extend the applicability of the SimGrid simulation framework from Grids and Peer-to-Peer systems to Clouds and High Performance Computation systems. Each type of large-scale computing system will be addressed through a set of use cases and lead by researchers recognized as experts in this area.

8.1.3. ADT - Inria Technological Development Actions

ADT SwLoc  (http://swloc.gforge.inria.fr/)
Participants: Raymond Namyst, Pierre-André Wacrenier, Andra Hugo, Brice Goglin, Corentin Salingue.
Inria ADT Campaign 2017, 10/2017 - 9/2019 (24 months)
Coordinator: Raymond Namyst
Abstract: The Inria action ADT SwLoc has the aim to develop a new library allowing dynamic flexible partitioning of computing resources in order to execute parallel regions.

8.1.4. IPL - Inria Project Lab

C2S@Exa - Computer and Computational Sciences at Exascale  Participant: Olivier Aumage.
Inria IPL 2013 - 2017 (48 months)
Coordinator: Stéphane Lantéri (team Nachos, Inria Sophia)
Since January 2013, the team is participating to the C2S@Exa http://www-sop.inria.fr/c2s_at_exa Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. This collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

HAC-SPECIS - High-performance Application and Computers, Studying PErformance and Correctness In Simulation
Participants: Samuel Thibault, Luka Stanisic, Emmanuelle Saillard.
Inria IPL 2016 - 2020 (48 months)
Coordinator: Arnaud Legrand (team Polaris, Inria Rhône Alpes)

Since June 2016, the team is participating to the HAC-SPECIS http://hacspecis.gforge.inria.fr/ Inria Project Lab (IPL). This national initiative aims at answering methodological needs of HPC application and runtime developers and allowing to study real HPC systems both from the correctness and performance point of view. To this end, it gathers experts from the HPC, formal verification and performance evaluation community.

8.2. European Initiatives

8.2.1. FP7 & H2020 Projects

8.2.1.1. INTERTWINE
Title: Programming Model INTERoperability ToWards Exascale
Programm: H2020
Duration: October 2015 - October 2018
Coordinator: EPCC
Partners:
- Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)
- Deutsches Zentrum für Luft - und Raumfahrt Ev (Germany)
- Fraunhofer Gesellschaft Zur Forderung Der Angewandten Forschung Ev (Germany)
- Institut National de Recherche en Informatique et en Automatique (France)
- Kungliga Tekniska Hoegskolan (Sweden)
- T-Systems Solutions for Research (Germany)
- The University of Edinburgh (United Kingdom)
- Universitat Jaume I de Castellon (Spain)
- The University of Manchester (United Kingdom)

Inria contact: Olivier Aumage

This project addresses the problem of programming model design and implementation for the Exascale. The first Exascale computers will be very highly parallel systems, consisting of a hierarchy of architectural levels. To program such systems effectively and portably, programming APIs with efficient and robust implementations must be ready in the appropriate timescale. A single, “silver bullet” API which addresses all the architectural levels does not exist and seems very unlikely to emerge soon enough. We must therefore expect that using combinations of different APIs at different system levels will be the only practical solution in the short to medium term. Although there remains
room for improvement in individual programming models and their implementations, the main challenges lie in interoperability between APIs. It is this interoperability, both at the specification level and at the implementation level, which this project seeks to address and to further the state of the art. INTERTWinE brings together the principal European organisations driving the evolution of programming models and their implementations. The project will focus on seven key programming APIs: MPI, GASPI, OpenMP, OmpSs, StarPU, QUARK and PaRSEC, each of which has a project partner with extensive experience in API design and implementation. Interoperability requirements, and evaluation of implementations will be driven by a set of kernels and applications, each of which has a project partner with a major role in their development. The project will implement a co-design cycle, by feeding back advances in API design and implementation into the applications and kernels, thereby driving new requirements and hence further advances.

8.2.1.2. Mont-Blanc 2

Title: Mont-Blanc
Programm: FP7
Coordinator: BSC
Partners:

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)
Atos/Bull (France)
ARM (United Kingdom)
Jülich (Germany)
LRZ (Germany)
University of Stuttgart (Germany)
CINECA (Italy)
CNRS (France)
CEA (France)
University of Bristol (United Kingdom)
Allinea Software (United Kingdom)
University of Cantabria (Spain)

Inria contact: Olivier Aumage

The Mont-Blanc project aims to develop a European Exascale approach leveraging on commodity power-efficient embedded technologies. The project has developed a HPC system software stack on ARM, and will deploy the first integrated ARM-based HPC prototype by 2014, and is also working on a set of 11 scientific applications to be ported and tuned to the prototype system.

8.2.2. Collaborations in European Programs, Except FP7 & H2020

Program: PRACE
Project acronym: PRACE-5IP
Project title: PRACE Fifth Implementation Phase
Duration: 01/2017
Coordinator: PRACE

Abstract: The objectives of PRACE-5IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. These include:

- assisting the transition to PRACE2 including analysis of TransNational Access;
• strengthening the internationally recognised PRACE brand;
• continuing and extend advanced training which so far provided more than 18 800 person-
training days;
• preparing strategies and best practices towards Exascale computing;
• coordinating and enhancing the operation of the multi-tier HPC systems and services;
• supporting users to exploit massively parallel systems and novel architectures.

A high level Service Catalogue is provided. The proven project structure will be used to achieve
each of the objectives in 6 dedicated work packages. The activities are designed to increase Europe’s
research and innovation potential especially through:
• seamless and efficient Tier-0 services and a pan-European HPC ecosystem including
  national capabilities;
• promoting take-up by industry and new communities and special offers to SMEs;
• implementing a new flexible business model for PRACE 2;
• proposing strategies for deployment of leadership systems;
• collaborating with the ETP4HPC, CoEs and other European and international organisa-
  tions on future architectures, training, application support and policies.

Inria contact for team STORM: Olivier Aumage

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. Member of the Organizing Committees
  • Samuel Thibault has organized a workshop panel at HCW’17

9.1.2. Scientific Events Selection

9.1.2.1. Chair of Conference Program Committees
  • Denis Barthou has been Chair of EuroPar 2017

9.1.2.2. Member of the Conference Program Committees
  • Denis Barthou has been Program Committee member of Europar 2017, UCHPC’17, HPCS’17, PACT’17
  • Olivier Aumage has been Program Committee member of the Cluster 2017 conference.
  • Samuel Thibault has been Program Committee member of P3MA’17, HCW’17, EuroPar 2017, ComPAS’2017.
  • Raymond Namyst has been Program Committee member of PPAM’17, SC’17 and EuroMPI/USA’17.

9.1.2.3. Reviewer

STORM members have conducted wide reviewing activities for the following conferences and workshops:
CCGRID, Cluster, EuroMPI, P3MA, PDSEC, HCW, Compas.

9.1.3. Journal

9.1.3.1. Reviewer - Reviewing Activities

STORM members have conducted reviewing activities for the following journals: IEEE TPDS, GPAA IJPEDS,
PARCO, Scientific Programming, JPDC
9.1.4. Invited Talks

- Denis Barthou has been invited at the PASC conference mini-symposium titled "From linear algebra to High performance code", 26/06/2017 Lugano.
- Denis Barthou has been invited at a Bird of Feather session at SC conference, 2017-11.
- Olivier Aumage has been invited at the special day event ‘Runtimes’ organized by Group ‘Calcul’ from CNRS (2017/01/20, PARIS).
- Samuel Thibault has been invited at the "Journées Scientifiques Inria 2017”.
- Samuel Thibault has been invited at the HPC Workshop at Total (2017-06-29, Pau).
- Samuel Thibault has been invited at the JLESC workshop (2017-07-20, Urbana-Champaign, US).
- Samuel Thibault has been invited at the "École thématique GPU" (2017-11-09, Grenoble).
- Raymond Namyst has been invited to the Dagstuhl Seminar on Performance Portability in Extreme Scale Computing: Metrics, Challenges, Solutions (2017-10, Schloss Dagstuhl, Germany).

9.1.5. Scientific Expertise

- Olivier Aumage represents Inria at the OpenMP ARB consortium of standardization for the OpenMP language.
- Samuel Thibault participates to the HiHAT working group.
- Raymond Namyst is member of the Khronos OpenCL advisory panel.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence: Samuel Thibault is responsible for the computer science topic of the first university semester.
Licence: Samuel Thibault is responsible for the creation of the new Licence Pro ADSILLH (Administrateur et Développeur de Systèmes Informatiques sous Licences Libres et Hybrides).
Licence: Samuel Thibault, Introduction to Computer Science, 32HeTD, L1, University of Bordeaux.
Licence: Samuel Thibault, Networking, 80HeTD, L3, University of Bordeaux.
Licence: Samuel Thibault, Tutored project, 5HeTD, L3, University of Bordeaux.
Licence: Marie-Christine Counilh, Introduction to Computer Science, 64HeTD, L1, University of Bordeaux.
Licence: Marie-Christine Counilh, Introduction to C programming, 52HeTD, L1, University of Bordeaux.
Master MIAGE: Marie-Christine Counilh, Object oriented programming in Java, 30HeTD, M1, University of Bordeaux.
Master: Marie-Christine Counilh, Internship supervision, 4HeTD, M2, University ob Bordeaux.
Engineering School: Emmanuelle Saillard, Structures arborescentes, 16HeTD, L3, ENSEIRB-MATMECA.
Engineering School: Pierre Huchant, Projet d’algorithmique et de programmation, 30HeTD, L3, ENSEIRB-MATMECA.
Engineering School: Pierre Huchant, Programmation Systeme, 18HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Pierre Huchant, Compilation, 14HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Pierre Huchant, Projet de Compilation, 4HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Olivier Aumage, High Performance Communication Libraries, 20HeTD, M2, ENSEIRB-MATMECA.
Engineering School: Olivier Aumage, Languages and Supports for Parallelism, 14HeTD, M2, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, Parallel architectures, 24HeTD, M2, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, 3D synthesis in real time, 35HeTD, M2, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, Architecture, 50HeTD, L3, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, Tutored project, 25HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, Compilation, 28HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, Compilation, 28HeTD, M1, ENSEIRB-MATMECA.
Engineering School: Denis Barthou, C project, 30HeTD, L3, ENSEIRB-MATMECA.

Engineering School: Denis Barthou was responsible till Sept 2017 of a 3rd year specialization in cybersecurity, system and network (M2) at ENSEIRB-MATMECA, certified by the ANSSSI. From Sept 2017, he is responsible of the computer science teaching department of ENSEIRB-MATMECA.

Licence: Pierre-André Wacrenier, Introduction to Computer Science, 64HeTD, L1, University of Bordeaux.
Licence: Pierre-André Wacrenier, System programming, 32HeTD, L3, University of Bordeaux
Master: Pierre-André Wacrenier, Parallel programming, 48HeTD, M1, University of Bordeaux
Master: Pierre-André Wacrenier is responsible for the Master’s Degree with specialization in HPC, M2, University of Bordeaux

University of Bordeaux: Raymond Namyst is vice-chair of the computer science training department
Licence: Raymond Namyst, UNIX programming, 54HeTD, L3, University of Bordeaux
Master: Raymond Namyst, Operating Systems, 60HeTD, M1, University of Bordeaux
Master: Raymond Namyst, Parallel programming, 33HeTD, M1, University of Bordeaux
Engineering School: Raymond Namyst, Microprocessors, 24HeTD, L3, ENSEIRB-MATMECA

Engineering School: Raymond Namyst, Parallel programming, 33HeTD, M1, ENSEIRB-MATMECA

9.2.2. Supervision

PhD in progress: Pierre Huchant, October 2015, M.-C. Counilh, D.Barthou and R. Namyst
PhD in progress: Adrien Cassagne, October 2017, O. Aumage, D. Barthou, C. Jego and C. Leroux
PhD in progress: Léo Villeveygoux, October 2017, R. Namyst
PhD in progress: Terry Cojean, October 2014, P.-A. Wacrenier and R. Namyst
PhD in progress: Hugo Brunie, October 2015, J. Jaeger, P. Carribault and D. Barthou
PhD in progress: Raphael Prat, October 2017, R. Namyst
PhD in progress: Arthur Lousseert, October 2015, J. Jaeger, P. Carribault and R. Namyst
PhD: Christopher Haine, January 2014-June 2017, O. Aumage and D. Barthou
PhD: Marc Sergent, Passage à l’échelle d’un support d’exécution à base de tâches pour l’algèbre linéaire dense, October 2014-January 2017, O. Aumage, S. Thibault and R. Namyst
PhD: Suraj Kumar, Scheduling of Dense Linear Algebra Kernels on Heterogeneous Resources, Université de Bordeaux, April 2017, E. Agullo, O. Beaumont, L. Eyraud, S. Thibault

9.2.3. Juries

Denis Barthou has participated to the following PhD/HDR juries
Nabil Hallou, PhD, U.Rennes, dec. 2017 (reviewer)
Abdou Guermouche, HDR, U. Bordeaux, dec. 2017 (member)
Raymond Namyst has participated to the following PhD/HDR committees:
- Sébastien Gougeaud, PhD, U. Versailles Saint-Quentin, may 2017 (reviewer)
- Yunsong Wang, PhD, Ecole Polytechnique, dec. 2017 (reviewer)
- Pierre Ramet, HDR, U. Bordeaux, dec. 2017 (member)

9.3. Popularization
- Séminaire Inria Bordeaux Sud-Ouest, Unithé ou Café, septembre 2017 sur la programmation parallèle (D. Barthou)
- Fête de la Science à l’Inria Bordeaux Sud-Ouest, ateliers Datagramme et Digit’elles, octobre 2017 (E. Saillard)
- Fête de la Science, ateliers Datagramme et Sciences Manuelles du Numérique, octobre 2017 (Y. Khorsi et C. Salingue)
- Printemps de la Mixité, atelier Datagramme, avril 2017 (C. Salingue)
- J’ai un bug, qu’est-ce que je peux faire ?, Mars 2017 (S. Thibault)
- Mon code en 180 secondes: StarPU+KStar, Journées SED Bordeaux, October 2017 (O. Aumage)

10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


International Conferences with Proceedings


Research Reports


Other Publications


References in notes


Project-Team TADaaM

Topology-aware system-scale data management for high-performance computing

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing
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Project-Team TADaaM

Creation of the Team: 2015 January 01, updated into Project-Team: 2017 December 01

Keywords:

Computer Science and Digital Science:
- A1.1.1. - Multicore, Manycore
- A1.1.2. - Hardware accelerators (GPGPU, FPGA, etc.)
- A1.1.3. - Memory models
- A1.1.4. - High performance computing
- A1.1.5. - Exascale
- A1.1.9. - Fault tolerant systems
- A1.2. - Networks
- A2.1.7. - Distributed programming
- A2.2.2. - Memory models
- A2.2.3. - Run-time systems
- A2.2.4. - Parallel architectures
- A2.6.1. - Operating systems
- A2.6.2. - Middleware
- A3.1.2. - Data management, querying and storage
- A3.1.3. - Distributed data
- A3.1.8. - Big data (production, storage, transfer)
- A6.2.6. - Optimization
- A6.2.7. - High performance computing
- A6.3.3. - Data processing
- A7.1.1. - Distributed algorithms
- A7.1.2. - Parallel algorithms
- A7.1.3. - Graph algorithms
- A8.1. - Discrete mathematics, combinatorics
- A8.2. - Optimization
- A8.7. - Graph theory
- A8.9. - Performance evaluation

Other Research Topics and Application Domains:
- B6.3.2. - Network protocols
- B6.3.3. - Network Management
- B6.5. - Information systems
- B9.4.1. - Computer science
- B9.6. - Reproducibility

1. Personnel

Research Scientists
Emmanuel Jeannot [Team leader, Inria, Senior Researcher, HDR]
2. Overall Objectives

2.1. Overall Objectives

In TADAAM, we propose a new approach where we allow the application to explicitly express its resource needs about its execution. The application needs to express its behavior, but in a different way from the compute-centric approach, as the additional information is not necessarily focused on computation and on instructions execution, but follows a high-level semantics (needs of large memory for some processes, start of a communication phase, need to refine the granularity, beginning of a storage access phase, description of data affinity, etc.). These needs will be expressed to a service layer though an API. The service layer will be system-wide (able to gather a global knowledge) and stateful (able to take decision based on the current request but also on previous ones). The API shall enable the application to access this service layer through a well-defined set of functions, based on carefully designed abstractions.

Hence, the goal of TADAAM is to design a stateful system-wide service layer for HPC systems, in order to optimize applications execution according to their needs.

This layer will abstract low-level details of the architecture and the software stack, and will allow applications to register their needs. Then, according to these requests and to the environment characteristics, this layer will feature an engine to optimize the execution of the applications at system-scale, taking into account the gathered global knowledge and previous requests.
This approach exhibits several key characteristics:

- It is independent from the application parallelization, the programming model, the numerical scheme and, largely, from the data layout. Indeed, high-level semantic requests can easily be added to the application code after the problem has been modeled, parallelized, and most of the time after the data layout has been designed and optimized. Therefore, this approach is – to a large extent – orthogonal to other optimization mechanisms and does not require application developers to rewrite their code.
- Application developers are the persons who know best their code and therefore the needs of their application. They can easily (if the interface is well designed and the abstractions are correctly exposed), express the application needs in terms of resource usage and interaction with the whole environment.
- Being stateful and shared by all the applications in the parallel environment, the proposed layer will therefore enable optimizations that:
  - cannot be performed statically but require information only known at launch- or run-time,
  - are incremental and require minimal changes to the application execution scheme,
  - deal with several parts of the environment at the same time (e.g., batch scheduler, I/O, process manager and storage),
  - take into account the needs of several applications at the same time and deal with their interaction. This will be useful, for instance, to handle network contention, storage access or any other shared resources.

3. Research Program

3.1. Need for System-Scale Optimization

Firstly, in order for applications to make the best possible use of the available resources, it is impossible to expose all the low-level details of the hardware to the program, as it would make impossible to achieve portability. Hence, the standard approach is to add intermediate layers (programming models, libraries, compilers, runtime systems, etc.) to the software stack so as to bridge the gap between the application and the hardware. With this approach, optimizing the application requires to express its parallelism (within the imposed programming model), organize the code, schedule and load-balance the computations, etc. In other words, in this approach, the way the code is written and the way it is executed and interpreted by the lower layers drives the optimization. In any case, this approach is centered on how computations are performed. Such an approach is therefore no longer sufficient, as the way an application is executing does depend less and less on the organization of computation and more and more on the way its data is managed.

Secondly, modern large-scale parallel platforms comprise tens to hundreds of thousand nodes. However, very few applications use the whole machine. In general, an application runs only on a subset of the nodes. Therefore, most of the time, an application shares the network, the storage and other resources with other applications running concurrently during its execution. Depending on the allocated resources, it is not uncommon that the execution of one application interferes with the execution of a neighboring one.

Lastly, even if an application is running alone, each element of the software stack often performs its own optimization independently. For instance, when considering an hybrid MPI/OpenMP application, one may realize that threads are concurrently used within the OpenMP runtime system, within the MPI library for communication progression, and possibly within the computation library (BLAS) and even within the application itself (pthreads). However, none of these different classes of threads are aware of the existence of the others. Consequently, the way they are executed, scheduled, prioritized does not depend on their relative roles, their locations in the software stack nor on the state of the application.

\(^0\)More than 22,500 XE6 compute node for the BlueWaters system; 5040 B510 Bullx Nodes for the Curie machine; more than 49,000 BGQ nodes for the MIRA machine.

\(^0\)In 2014, the median case was 2048 nodes for the BlueWaters system and, for the first year of the Curie machine, the median case was 256 nodes.
The above remarks show that in order to go beyond the state-of-the-art, it is necessary to design a new set of mechanisms allowing cross-layer and system-wide optimizations so as to optimize the way data is allocated, accessed and transferred by the application.

### 3.2. Scientific Challenges and Research Issues

In TADAAM, we will tackle the problem of efficiently executing an application, at system-scale, on an HPC machine. We assume that the application is already optimized (efficient data layout, use of effective libraries, usage of state-of-the-art compilation techniques, etc.). Nevertheless, even a statically optimized application will not be able to be executed at scale without considering the following dynamic constraints: machine topology, allocated resources, data movement and contention, other running applications, access to storage, etc. Thanks to the proposed layer, we will provide a simple and efficient way for already existing applications, as well as new ones, to express their needs in terms of resource usage, locality and topology, using a high-level semantic.

It is important to note that we target the optimization of each application independently but also several applications at the same time and at system-scale, taking into account their resource requirement, their network usage or their storage access. Furthermore, dealing with code-coupling application is an intermediate use-case that will also be considered.

Several issues have to be considered. The first one consists in providing relevant abstractions and models to describe the topology of the available resources and the application behavior. Therefore, the first question we want to answer is: “How to build scalable models and efficient abstractions enabling to understand the impact of data movement, topology and locality on performance?” These models must be sufficiently precise to grasp the reality, tractable enough to enable efficient solutions and algorithms, and simple enough to remain usable by non-hardware experts. We will work on (1) better describing the memory hierarchy, considering new memory technologies; (2) providing an integrated view of the nodes, the network and the storage; (3) exhibiting qualitative knowledge; (4) providing ways to express the multi-scale properties of the machine. Concerning abstractions, we will work on providing general concepts to be integrated at the application or programming model layers. The goal is to offer means, for the application, to express its high-level requirements in terms of data access, locality and communication, by providing abstractions on the notion of hierarchy, mesh, affinity, traffic metrics, etc.

In addition to the abstractions and the aforementioned models we need to define a clean and expressive API in a scalable way, in order for applications to express their needs (memory usage, affinity, network, storage access, model refinement, etc.). Therefore, the second question we need to answer is: “how to build a system-scale, stateful, shared layer that can gather applications needs expressed with a high-level semantic?”. This work will require not only to define a clean API where applications will express their needs, but also to define how such a layer will be shared across applications and will scale on future systems. The API will provide a simple yet effective way to express different needs such as: memory usage of a given portion of the code; start of a compute intensive part; phase where the network is accessed intensively; topology-aware affinity management; usage of storage (in read and/or write mode); change of the data layout after mesh refinement, etc. From an engineering point of view, the layer will have a hierarchical design matching the hardware hierarchy, so as to achieve scalability.

Once this has been done, the service layer, will have all the information about the environment characteristics and application requirements. We therefore need to design a set of mechanisms to optimize applications execution: communication, mapping, thread scheduling, data partitioning/mapping/movement, etc.

Hence, the last scientific question we will address is: “How to design fast and efficient algorithms, mechanisms and tools to enable execution of applications at system-scale, in full a HPC ecosystem, taking into account topology and locality?” A first set of research is related to thread and process placement according to the topology and the affinity. Another large field of study is related to data placement, allocation and partitioning: optimizing the way data is accessed and processed especially for mesh-based applications. The issues of transferring data across the network will also be tackled, thanks to the global knowledge we
have on the application behavior and the data layout. Concerning the interaction with other applications, several directions will be tackled. Among these directions we will deal with matching process placement with resource allocation given by the batch scheduler or with the storage management: switching from a best-effort application centric strategy to global optimization scheme.

4. Application Domains

4.1. Mesh-based applications

TADAAM targets scientific simulation applications on large-scale systems, as these applications present huge challenges in terms of performance, locality, scalability, parallelism and data management. Many of these HPC applications use meshes as the basic model for their computation. For instance, PDE-based simulations using finite differences, finite volumes, or finite elements methods operate on meshes that describe the geometry and the physical properties of the simulated objects. This is the case for at least two thirds of the applications selected in the 9th PRACE call 0, which concern quantum mechanics, fluid mechanics, climate, material physics, electromagnetism, etc.

Mesh-based applications not only represent the majority of HPC applications running on existing supercomputing systems, yet also feature properties that should be taken into account to achieve scalability and performance on future large-scale systems. These properties are the following:

- **Size**: Datasets are large: some meshes comprise hundreds of millions of elements, or even billions.
- **Dynamicity**: In many simulations, meshes are refined or coarsened at each time step, so as to account for the evolution of the physical simulation (moving parts, shockwaves, structural changes in the model resulting from collisions between mesh parts, etc.).
- **Structure**: Many meshes are unstructured, and require advanced data structures so as to manage irregularity in data storage.
- **Topology**: Due to their rooting in the physical world, meshes exhibit interesting topological properties (low dimensionality embedding, small maximum degree, large diameter, etc.). It is very important to take advantage of these properties when laying out mesh data on systems where communication locality matters.

All these features make mesh-based applications a very interesting and challenging use-case for the research we want to carry out in this project. Moreover, we believe that our proposed approach and solutions will contribute to enhance these applications and allow them to achieve the best possible usage of the available resources of future high-end systems.

5. Highlights of the Year

5.1. Highlights of the Year

Guillaume Aupy was the Technical Program vice-chair of SC’17. This is the main conference of the field gathering more than 12,700 attendees (practitioners, industrials and researchers) from 79 different nationalities. It is the first time someone from Inria is in charge of the technical program in 30 years of the conference. The Technical Program of SC17 comprises of 13 different elements (papers, workshops, panels, invited talks etc), for a total of 880 submissions from about 2900 unique individuals! 370 different volunteers participated in the review process of one or multiple elements of the Technical Program.

0 http://www.prace-ri.eu/prace-9th-regular-call/
6. New Software and Platforms

6.1. Hsplit

Hierarchical communicators split

KEYWORDS: MPI communication - Topology - Hardware platform

SCIENTIFIC DESCRIPTION: Hsplit is a library that implements an abstraction allowing the programmer using MPI in their parallel applications to access the underlying hardware structure through a hierarchy of communicators. Hsplit is based on the MPI_Comm_split_type routine and provides a new value for the split_type argument that specifically creates a hierarchy a subcommunicators where each new subcommunicator corresponds to a meaningful hardware level. The important point is that only the structure of the hardware is exploited and the number of levels or the levels names are not fixed so as to propose a solution independent from future hardware evolutions (such as new levels for instance). Another flavor of this MPI_Comm_split_type function is provided that creates a roots communicators at the same time a subcommunicator is produced, in order to ease the collective communication and/or synchronization among subcommunicators.

FUNCTIONAL DESCRIPTION: Hsplit implements an abstraction that allows the programmer using MPI in their parallel applications to access the underlying hardware structure through a hierarchy of communicators. Hsplit is based on the MPI_Comm_split_type routine and provides a new value for the split_type argument that specifically creates a hierarchy a subcommunicators where each new subcommunicator corresponds to a meaningful hardware level. The important point is that only the structure of the hardware is exploited and the number of levels or the levels names are not fixed so as to propose a solution independent from future hardware evolutions (such as new levels for instance). Another flavor of this MPI_Comm_split_type function is provided that creates a roots communicators at the same time a subcommunicator is produced, in order to ease the collective communication and/or synchronization among subcommunicators.

NEWS OF THE YEAR: A new working group in the MPI Forum to champion the integration of this proposal in the MPI standard has been created. This working group includes Inria, CEA, Atos/Bull, Paratools, the University of Tennessee - Knoxville and many other institutions/companies are interested to join in.

- Participants: Guillaume Mercier, Brice Goglin, Emmanuel Jeannot and Farouk Mansouri
- Contact: Guillaume Mercier
- Publications: A hierarchical model to manage hardware topology in MPI applications - A Hierarchical Model to Manage Hardware Topology in MPI Applications
- URL: http://mpi-topology.gforge.inria.fr/

6.2. hwloc

Hardware Locality

KEYWORDS: NUMA - Multicore - GPU - Affinities - Open MPI - Topology - HPC - Locality

FUNCTIONAL DESCRIPTION: Hardware Locality (hwloc) is a library and set of tools aiming at discovering and exposing the topology of machines, including processors, cores, threads, shared caches, NUMA memory nodes and I/O devices. It builds a widely-portable abstraction of these resources and exposes it to applications so as to help them adapt their behavior to the hardware characteristics. They may consult the hierarchy of resources, their attributes, and bind task or memory on them.
hwloc targets many types of high-performance computing applications, from thread scheduling to placement of MPI processes. Most existing MPI implementations, several resource managers and task schedulers, and multiple other parallel libraries already use hwloc.

- Participants: Brice Goglin and Samuel Thibault
- Partners: Open MPI consortium - Intel - AMD
- Contact: Brice Goglin
- URL: http://www.open-mpi.org/projects/hwloc/

6.3. NetLoc

**Network Locality**

**KEYWORDS**: Topology - Locality - Distributed networks - HPC - Parallel computing - MPI communication

**FUNCTIONAL DESCRIPTION**: netloc (Network Locality) is a library that extends hwloc to network topology information by assembling hwloc knowledge of server internals within graphs of inter-node fabrics such as Infiniband, Intel OmniPath or Cray networks.

Netloc builds a software representation of the entire cluster so as to help applications properly place their tasks on the nodes. It may also help communication libraries optimize their strategies according to the wires and switches.

Netloc targets the same challenges as hwloc but focuses on a wider spectrum by enabling cluster-wide solutions such as process placement. It interoperates with the Scotch graph partitioner to do so.

Netloc is distributed within hwloc releases starting with hwloc 2.0.

- Participants: Brice Goglin, Clement Foyer and Cyril Bordage
- Contact: Brice Goglin
- URL: http://www.open-mpi.org/projects/netloc/

6.4. NewMadeleine

**KEYWORDS**: High-performance calculation - MPI communication

**FUNCTIONAL DESCRIPTION**: NewMadeleine is the fourth incarnation of the Madeleine communication library. The new architecture aims at enabling the use of a much wider range of communication flow optimization techniques. Its design is entirely modular: drivers and optimization strategies are dynamically loadable software components, allowing experimentations with multiple approaches or on multiple issues with regard to processing communication flows.

The optimizing scheduler SchedOpt targets applications with irregular, multi-flow communication schemes such as found in the increasingly common application conglomerates made of multiple programming environments and coupled pieces of code, for instance. SchedOpt itself is easily extensible through the concepts of optimization strategies (what to optimize for, what the optimization goal is) expressed in terms of tactics (how to optimize to reach the optimization goal). Tactics themselves are made of basic communication flows operations such as packet merging or reordering.
The communication library is fully multi-threaded through its close integration with PIOMan. It manages concurrent communication operations from multiple libraries and from multiple threads. Its MPI implementation Mad-MPI fully supports the MPI_THREAD_MULTIPLE multi-threading level.

- Participants: Alexandre Denis, Clement Foyer, Nathalie Furmento and Raymond Namyst
- Contact: Alexandre Denis
- URL: http://pm2.gforge.inria.fr/newmadeleine/

6.5. PaMPA

**Parallel Mesh Partitioning and Adaptation**

**KEYWORDS**: Dynamic load balancing - Unstructured heterogeneous meshes - Parallel remeshing - Subdomain decomposition - Parallel numerical solvers

**SCIENTIFIC DESCRIPTION**: PaMPA is a parallel library for handling, redistributing and remeshing unstructured meshes on distributed-memory architectures. PaMPA dramatically eases and speeds-up the development of parallel numerical solvers for compact schemes. It provides solver writers with a distributed mesh abstraction and an API to: - describe unstructured and possibly heterogeneous meshes, on the form of a graph of interconnected entities of different kinds (e.g. elements, faces, edges, nodes), - attach values to the mesh entities, - distribute such meshes across processing elements, with an overlap of variable width, - perform synchronous or asynchronous data exchanges of values across processing elements, - describe numerical schemes by means of iterators over mesh entities and their connected neighbors of a given kind, - redistribute meshes so as to balance computational load, - perform parallel dynamic remeshing, by applying adequately a user-provided sequential remesher to relevant areas of the distributed mesh.

PaMPA runs concurrently multiple sequential remeshing tasks to perform dynamic parallel remeshing and redistribution of very large unstructured meshes. E.g., it can remesh a tetrahedral mesh from 43M elements to more than 1Belements on 280 Broadwell processors in 20 minutes.

**FUNCTIONAL DESCRIPTION**: Parallel library for handling, redistributing and remeshing unstructured, heterogeneous meshes on distributed-memory architectures. PaMPA dramatically eases and speeds-up the development of parallel numerical solvers for compact schemes.

**NEWS OF THE YEAR**: PaMPA has been used to remesh an industrial mesh of a helicopter turbine combustion chamber, up to more than 1 billion elements.

- Participants: Cécile Dobrzynski, Cedric Lachat and François Pellegrini
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Cedric Lachat
- URL: http://project.inria.fr/pampa/

6.6. TreeMatch

**KEYWORDS**: Intensive parallel computing - High-Performance Computing - Hierarchical architecture - Placement

**SCIENTIFIC DESCRIPTION**: TreeMatch embeds a set of algorithms to map processors/cores in order to minimize the communication cost of the application.

Important features are : the number of processors can be greater than the number of applications processes , it assumes that the topology is a tree and does not require valuation of the topology (e.g. communication speeds) , it implements different placement algorithms that are switched according to the input size.

Some core algorithms are parallel to speed-up the execution. Optionally embeds scotch for fix-vertex mapping, enable exhaustive search if required. Several metric mapping are computed. Allow for oversubscribing of ressources. multithreaded.

TreeMatch is integrated into various software such as the Charm++ programming environment as well as in both major open-source MPI implementations: Open MPI and MPICH2.
**FUNCTIONAL DESCRIPTION:** TreeMatch is a library for performing process placement based on the topology of the machine and the communication pattern of the application.
- **Participants:** Adele Villiermet, Emmanuel Jeannot, François Tessier, Guillaume Mercier and Pierre Celor
- **Partners:** Université de Bordeaux - CNRS - IPB
- **Contact:** Emmanuel Jeannot
- **URL:** http://treematch.gforge.inria.fr/

6.7. SCOTCH

**KEYWORDS:** Mesh partitioning - Domain decomposition - Graph algorithmics - High-performance calculation - Sparse matrix ordering

**FUNCTIONAL DESCRIPTION:** Scotch is a graph partitioner. It helps optimise the division of a problem, by means of a graph, into a set of independent sub-problems of equivalent sizes. These sub-problems can also be solved at the same time.

**RELEASE FUNCTIONAL DESCRIPTION:** Version 6.0 offers many new features:
- sequential graph repartitioning
- sequential graph partitioning with fixed vertices
- new, fast, direct k-way partitioning and mapping algorithms
- multi-threaded, shared memory algorithms in the (formerly) sequential part of the library
- exposure in the API of many distributed graph handling routines
- embedded pseudo-random generator for improved reproducibility

**NEWS OF THE YEAR:** In the context of the PhD of Rémi Barat, the sequential version of Scotch has been extended so as to manage graphs with multiple vertex weights, and multi-constraint graph partitioning algorithms have been implemented as prototypes.
- **Participants:** Sébastien Fourestier, François Pellegrini and Cédric Chevalier
- **Partners:** CNRS - IPB - Region Aquitaine
- **Contact:** François Pellegrini

**URL:** http://www.labri.fr/~pelegrin/scotch/

7. New Results

7.1. Network Modeling

**NETLOC** (see Section 6.3) is a tool in HWLOC to discover the network topology. The information gathered and analysed are now saved in XML format. It brings more flexibility, readability and compatibility. Henceforth, in the display tool, we compute the positions of the nodes rather than use physics algorithm provided by vis.js library for node placement. Thus, it makes the visualization faster and we can display a fat-tree with around 41k nodes in less than 1 second.
Moreover, we can deal with other kinds of topologies. We handle topologies in a generic way and can have nested topologies. For the mapping, we build a deco graph in SCOTCH. Consequently, the mapping will be possible for any architecture. \[17\]

We have also optimized the mapping by giving a preconditioned matrix to SCOTCH, and by computing some metrics in order to evaluate mappings and keep the best one.

The part about discovering network have been improved and we support now, in addition to Infiniband, Omnipath fat-trees, Cray Torus.

7.2. Locality Aware Roofline Model

The trend of increasing the number of cores on-chip is enlarging the gap between compute power and memory performance. This issue leads to design systems with heterogeneous memories, creating new challenges for data locality. Before the release of those memory architectures, the Cache-Aware Roofline Model [47] (CARM) offered an insightful model and methodology to improve application performance with knowledge of the cache memory subsystem.

With the help of hwloc library, we are able to leverage the machine topology to extend the CARM for modeling NUMA and heterogeneous memory systems, by evaluating the memory bandwidths between all combinations of cores and NUMA nodes. The new Locality Aware Roofline Model [19] (LARM) scopes most contemporary types of large compute nodes and characterizes three bottlenecks typical of those systems, namely contention, congestion and remote access.

This work has been achieved in collaboration with the authors of the CARM and the source code of the associated tool is publicly available at https://github.com/NicolasDenoyelle/Locality-Aware-Roofline-Model.

In the future we plan to design and embed in the model an hybrid memory bandwidth model to provide an automatic roof matching feature.

7.3. Scalable Management of Platform Topologies

HWLOC (see Section 6.2) is used for gathering the topology of computing nodes. Those nodes are now growing to hundreds of cores, making the overall amount of topology information non-negligible. We studied the overhead of topology discovery on the overall execution time and showed that the Linux kernel is bottleneck on large nodes. It raised the need to use exported and/or abstracted topologies to factorize this overhead [22].

The memory footprint of locality information is also becoming an issue on large many-core. We designed a way to share this information between processes inside nodes so as to factorize this memory consumption [45].

7.4. New algorithm for I/O scheduling

We started working on I/O scheduling for HPC applications. HPC applications can be caracterized by I/O patterns that are repeated periodically. We showed in a simple context how this information can be taken into account to outperform state of the art I/O schedulers [15].

These preliminary results led to the obtention of the ANR DASH (see Section 9.1.2).

After which, we have performed a theoretical analysis to show how one should size the burst-buffers and the bandwidth to those buffers on a HPC system depending on the applications running. In our study we focused on one role of the buffers (namely the role of buffer to the PFS) [42]. This study is particularly important since those buffers are limited and can be used for many usage. Over or under booking the buffers for a specific use leads to an increase of congestion.
7.5. Topology-Aware Data Aggregation on Large-Scale Supercomputers

We have continued our work on two-phase I/O and data aggregation. This strategy consists of selecting a subset of processes to aggregate contiguous pieces of data before performing reads/writes. In collaboration with Argonne National Lab, we have worked on TAPIOCA, an MPI-based library implementing an efficient topology-aware two-phase I/O algorithm. TAPIOCA can take advantage of double-buffering and one-sided communication to reduce as much as possible the idle time during data aggregation. We also introduce our cost model leading to a topology-aware aggregator placement optimizing the movements of data. We validate our approach at large scale on two leadership-class supercomputers: Mira (IBM BG/Q) and Theta (Cray XC40). On BG/Q+GPFS, for instance, our algorithm leads to a performance improvement by a factor of twelve while on the Cray XC40 system associated with a Lustre filesystem, we achieve an improvement of four [27].


Process placement, also called topology mapping, is a well-known strategy to improve parallel program execution by reducing the communication cost between processes. It requires two inputs: the topology of the target machine and a measure of the affinity between processes. In the literature, the dominant affinity measure is the communication matrix that describes the amount of communication between processes. We have studied the accuracy of the communication matrix as a measure of affinity. We have done an extensive set of tests with two fat-tree machines and a 3d-torus machine to evaluate several hypotheses that are often made in the literature and to discuss their validity. First, we check the correlation between algorithmic metrics and the performance of the application. Then, we check whether a good generic process placement algorithm never degrades performance. And finally, we see whether the structure of the communication matrix can be used to predict gain.

7.7. Automatic, Abstracted and Portable Topology-Aware Thread Placement

Efficiently programming shared-memory machines is a difficult challenge because mapping application threads onto the memory hierarchy has a strong impact on the performance. However, optimizing such thread placement is difficult: architectures become increasingly complex and application behavior changes with implementations and input parameters, e.g. problem size and number of threads. We have worked on a fully automatic, abstracted and portable affinity module. It produces and implements an optimized affinity strategy that combines knowledge about application characteristics and the platform topology. Implemented in the back-end of our runtime system (ORWL), our approach was used to enhance the performance and the scalability of several unmodified ORWL-coded applications [23].

7.8. Process Placement with TreeMatch

We released TREEMATCH version 1.0 in June. The new feature are: a stabilize API, optional integration of SCOTCH, extensive testing of all the features.

7.9. Managing StarPU Communications with NewMadeleine

We have worked on the scalability with the number of communication requests in the NewMadeleine 6.4 communication library, so as to be able to manage communication patterns from the StarPU runtime. We have ported [44] StarPU on top of NewMadeleine so as to take benefit from NewMadeleine scalability in StarPU. Preliminary results are encouraging.
7.10. New abstraction to manage hardware topologies in MPI applications

Since the end of year 2016, we have been working on new abstractions and mechanisms that can allow the programmer to take advantage of the underlying hardware topology in their parallel applications developed in MPI. For instance, taking into account the intricate network/memory hierarchy can lead to substantial improvements in communication performance and reduce altogether the overall execution time of the application. However, it is important to find the relevant level of abstraction, as too much details are not usable practically because the programmer is not a hardware specialist most of the time. Also, MPI being hardware-agnostic, it is important to find means to use the hardware specifics without being tied to a particular architecture or hardware design.

With these goals in mind, we proposed the HSPLIT (see Section 6.1) library that implements a solution based on a well-known MPI concept, the communicators (that can be seen as groups of communicating processes). With HSPLIT, each level in the hardware hierarchy is accessible through a dedicated communicator. In this way, the programmer can leverage the underlying hierarchy in their application quite simply. The current implementation of HSPLIT is based on both HWLOC and NETLOC.

This work led to the creation of a new active working group within the MPI Forum, coordinated and lead by Inria.


Process placement, also called topology mapping, is a well-known strategy to improve parallel program execution by reducing the communication cost between processes. It requires two inputs: the topology of the target machine and a measure of the affinity between processes. In the literature, the dominant affinity measure is the communication matrix that describes the amount of communication between processes. We have studied the accuracy of the communication matrix as a measure of affinity. We have done an extensive set of tests with two fat-tree machines and a 3d-torus machine to evaluate several hypotheses that are often made in the literature and to discuss their validity. First, we check the correlation between algorithmic metrics and the performance of the application. Then, we check whether a good generic process placement algorithm never degrades performance. And finally, we see whether the structure of the communication matrix can be used to predict gain [35].

7.12. Gradient reconstruction in a legacy CFD application using task-based programming models

We investigated different runtime systems, namely StarPU and PaRSEC and their use in a legacy CFD code from EDF R&D. We assessed both runtimes in terms of performance, ease of implementation and various others criterion such as maintainability, documentation and team activity. By experimenting these solutions out of classical linear algebra problems, we push them out of their comfort zone into the common issues seen in Computational Fluid Dynamics codes with unstructured meshes [30].

7.13. Efficient multi-constraint graph partitioning algorithms

Although several tools provide multi-constraint graph partitioning features, this problem had not been thoroughly investigated. In the context of the PhD of Rémi Barat, several significant results were achieved regarding the multi-constraint graph partitioning problem.

Firstly, a theoretical analysis of the solution space of the mono-criterion, balanced graph bipartitioning problem showed that this space is strongly connected. Hence, local optimization algorithms may indeed succeed in finding paths to better solutions, from some existing solution. A conjecture on the multi-criteria case has been derived. These findings reversed our view on partitioning: while most tools try to find a possibly unbalanced partition of small cut, and then try to rebalance it, it is in fact possible to compute a balanced partition of arbitrary cut, and then to improve the cut.
Secondly, a thorough investigation of the multilevel framework, and of its implementations in several existing tools, allowed us to define the characteristics of an effective coarsening method, both in the mono-criterion and multi-criteria case. Also, new multi-criteria graph algorithms were designed for the initial partitioning and local optimization phases of the multilevel framework [43]. A new data structure has been devised, which speeds-up the computation of balanced partitions in the multi-criteria case.

Thirdly, all of the aforementioned algorithms were implemented in a prototype version of SCOTCH.

7.14. Progress threads placement for MPI Non-Blocking Collectives

MPI Non-Blocking Collectives (NBC) allow for communication overlap with computation. A good overlapping ratio is obtained when computation and communication are running in parallel. To achieve this, each MPI task generates a progress thread to manage communication tasks. The progression of these communications requires regular access to the processors. These threads compete with each other and with MPI tasks. In order to run threads with minimal disruption, we bound the progress threads on free cores when it is possible. Then, we showed that folding all progress threads on very few cores does not work for tree algorithms. The number of communication generated are too important. The solution that we propose is to perform a number of levels (S) of the dependency tree on MPI tasks. We get a reasonable execution time (less than compute time + communication time) while reserving fewer cores for progress threads. All these methods have been implemented in the MPC framework, which contributes to its development.

7.15. Use of PaMPA on large-scale simulations

Many improvements have been brought to PaMPA this year, to improve its robustness and scalability, and to extend its features. In the context of a joint work with CERFACS, PaMPA was subsequently used to remesh the mesh of a helicopter turbine combustion chamber, up to 1 billion elements. This allowed to run a Large-Eddy Simulation (LES) simulation that was out of reach of previous state-of-the-art remeshing software [38].

7.16. Co-scheduling applications on cache-partitioned systems

Cache-partitioned architectures allow subsections of the shared last-level cache (LLC) to be exclusively reserved for some applications. This technique dramatically limits interactions between applications that are concurrently executing on a multi-core machine. We have provided efficient algorithms to co-schedule multiple applications on cache-partitioned systems and evaluations showing that they performed well [13], [6]. We are currently in the process of evaluating them on real machines.

7.17. Dynamic memory-aware task-tree scheduling

We have provided new efficient algorithms that can be used for sparse matrices factorizations under memory constraints. We provide speedup of 15 to 45% over existing strategies and we are working on an actual implementation in QR-MUMPS [14].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

8.1.1. Intel

INTEL granted $30k and provided information about future many-core platforms and memory architectures to ease the design and development of the HWLOC software with early support for next generation hardware.

8.1.2. CEA

CEA is funding the PhD thesis of Hugo Taboada on specialized thread management in the context of multi programming models, and the PhD thesis of Rémi Barat on multi-criteria graph partitioning.
8.1.3. Bull/Atos

Bull/ATOS is granting the CIFRE PhD thesis on Nicolas Denoyelle on advanced memory hierarchies and new topologies.

8.1.4. EDF

EDF is granting the CIFRE PhD thesis of Benjamin Lorendeau on new programming models and optimization of Code Saturn.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. PIA ELCI, Environnement Logiciel pour le Calcul Intensif, 2014-2018

The ELCI PIA project is coordinated by BULL with several partners: CEA, Inria, SAFRAN, UVSQ.

This project aims to improve the support for numerical simulations and High Performance Computing (HPC) by providing a new generation software stack to control supercomputers, to improve numerical solvers, and pre- and post computing software, as well as programming and execution environment. It also aims at validating the relevance of these developments by demonstrating their capacity to deliver better scalability, resilience, modularity, abstraction, and interaction on some application use-cases. TADAAM is involved in WP1 and WP2 ELCI Work Packages. Emmanuel JEANNOT is the Inria representative in the ELCI steering committee.

9.1.2. ANR

ANR MOEBUS Scheduling in HPC (http://moebus.gforge.inria.fr/doku.php).

ANR INFRA 2013, 10/2013 - 9/2017 (48 months)
Coordinator: Denis Trystram (Inria Rhône-Alpes)
Other partners: Inria Bordeaux Sud-Ouest, Bull/ATOS
Abstract: This project focuses on the efficient execution of parallel applications submitted by various users and sharing resources in large-scale high-performance computing environments.


AP générique 2015, 01/2016 - 12-2019 (48 months)
Coordinator: Laurent Simon (LaBRI)
Other partners: CRIL (Univ. Artois), Inria Lille (Spirals)
Abstract: The SATAS project aims to advance the state of the art in massively parallel SAT solving. The final goal of the project is to provide a “pay as you go” interface to SAT solving services and will extend the reach of SAT solving technologies, daily used in many critical and industrial applications, to new application areas, which were previously considered too hard, and lower the cost of deploying massively parallel SAT solvers on the cloud.

ANR DASH Data-Aware Scheduling at Higher scale (https://project.inria.fr/dash/).

AP générique JCJC 2017, 03/2018 - 02-2022 (48 months)
Coordinator: Guillaume AUPY (Tadaam)
Abstract: This project focuses on the efficient execution of I/O for High-Performance applications. The idea is to take into account some knowledge on the behavior of the different I/O steps to compute efficient schedules, and to update them dynamically with the online information.
9.2. European Initiatives

9.2.1. Collaborations in European Programs, Except FP7 & H2020

COLOC: the Concurrency and Locality Challenge (http://www.coloc-itea.org).
- Program: ITEA2
- Project acronym: COLOC
- Project title: The Concurrency and Locality Challenge
- Duration: November 2014 - November 2017
- Coordinator: BULL/ATOS
- Other partners: BULL/ATOS (France); Dassault Aviation (France); Enfeild AB (Sweden); Scilab entreprise (France); Teratec (France); Inria (France); Swedish De芬bse Research Agency - FOI (France); UVSQ (France).
- Abstract: The COLOC project aims at providing new models, mechanisms and tools for improving applications performance and supercomputer resources usage taking into account data locality and concurrency.

NESUS: Network for Ultrascale Computing (http://www.nesia.eu)
- Program: COST
- Project acronym: NESUS
- Project title: Network for Ultrascale Computing
- Duration: April 2014 - April 2018
- Coordinator: University Carlos III de Madrid
- Other partners: more than 35 countries
- Abstract: Ultrascale systems are envisioned as large-scale complex systems joining parallel and distributed computing systems that will be two to three orders of magnitude larger that today's systems. The EU is already funding large scale computing systems research, but it is not coordinated across researchers, leading to duplications and inefficiencies. The goal of the NESUS Action is to establish an open European research network targeting sustainable solutions for ultrascale computing aiming at cross fertilization among HPC, large scale distributed systems, and big data management. The network will contribute to glue disparate researchers working across different areas and provide a meeting ground for researchers in these separate areas to exchange ideas, to identify synergies, and to pursue common activities in research topics such as sustainable software solutions (applications and system software stack), data management, energy efficiency, and resilience. Some of the most active research groups of the world in this area are members of this proposal. This Action will increase the value of these groups at the European-level by reducing duplication of efforts and providing a more holistic view to all researchers, it will promote the leadership of Europe, and it will increase their impact on science, economy, and society. Emmanuel JEANNOT is the vice-chair of this Action.

9.2.2. Collaborations with Major European Organizations
- Partner 1: INESC-ID, Lisbon, (Portugal)
- Subject 1: Application modeling for hierarchical memory system

9.3. International Initiatives

9.3.1. Inria International Labs

Joint-Lab on Extreme Scale Computing (JLESC):
- Coordinators: Franck Cappello (general) and Yves Robert (Inria coordinator).
Other partners: Argonne National Lab, University of Urbanna Champaign (NCSA), Tokyo Riken, Jülich Supercomputing Center, Barcelona Supercomputing Center (BSC).

Abstract: The purpose of the Joint Laboratory for Extreme Scale Computing (JLESC) is to be an international, virtual organization whose goal is to enhance the ability of member organizations and investigators to make the bridge between Petascale and Extreme computing. The founding partners of the JLESC are Inria and UIUC. Further members are ANL, BSC, JSC and RIKEN-AICS.

9.3.2. Inria International Partners

9.3.2.1. Informal International Partners

Partner 1: ICL at University of Tennessee
Subject 1: on instrumenting MPI applications and modeling platforms (works on HWLOC take place in the context of the OPEN MPI consortium) and MPI and process placement

Partner 2: Argonne National Lab
Subject 2: Topology-aware data aggregation for I/O intensive application

Partner 3: Vanderbilt University
Subject 3: Data-scheduling on hierarchical memories

9.4. Close cooperation with Industry

- Advanced Micro Devices, Inc. (AMD): AMD Zen micro-architecture and EPYC processors topology support in the Linux kernel.
- Oracle Corporation: Topology detection for SPARC processors and Solaris operating systems.
- ARM Holdings and Cavium, Inc.: ARM processor ACPI PPTT firmwares and Linux kernel topology information.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Aleksandar Ilic from University of Lisbon visited us to continue our collaboration on the Locality-aware Roofline Model [19].
- Tobias Fuchs from Ludwig-Maximilians-University of Munich visited us to improve the use of hardware locality in the DYLOC runtime system.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair
Guillaume AUPY was the technical program vice-chair of SC’17.

10.1.1.2. Member of the steering committee
Emmanuel JEANNOT is member of the steering committee of Euro-Par and the Cluster international conference.
10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees
- Guillaume AUPY was the Parallel and Distributed algorithm area co-chair of ICA3PP’17.
- Guillaume AUPY is the chair of the Workshop committee of SC’18.

10.1.2.2. Member of the Conference Program Committees
- Brice GOGLIN was a member of the program committee of EuroMPI/USA 2017, HotInterconnect 25, CARLA 2017, and of the Exacomm ISC workshop and COLOC Euro-Par workshop.
- Guillaume AUPY was a member of the program committee of ICPP’17, SC’17, FTS’17.
- Alexandre DENIS was a member of the program committee of CCGrid 2017, HiPC 2017, Com-Pas’2017, CCGrid 2018.
- Guillaume AUPY was the Parallel and Distributed algorithm area co-chair of ICA3PP’17.
- Emmanuel JEANNOT was the Open workshop on data locality workshop co-chair in conjunction with Euro-Par 2017.
- Emmanuel JEANNOT was the Heterogeneity in Computing Workshop (HCW) chair in conjunction with IPDPS 2017.

10.1.2.3. Member of the Conference Program Committees
- Brice GOGLIN was a member of the program committee of EuroMPI/USA 2017, HotInterconnect 25, CARLA 2017, and of the Exacomm ISC workshop and COLOC Euro-Par workshop.
- Guillaume AUPY was a member of the program committee of ICPP’17, SC’17, FTS’17.
- Alexandre DENIS was a member of the program committee of CCGrid 2017, HiPC 2017, Com-Pas’2017, CCGrid 2018.
- Emmanuel JEANNOT was member of the program committee of SBAC-PAD 2017, HiPC 2017, ICPP 2017, Heteropar 2017, IPDPS 2018.
- Guillaume AUPY was the Parallel and Distributed algorithm area co-chair of ICA3PP’17.

10.1.2.4. Member of the Conference Program Committees
- Brice GOGLIN was a member of the program committee of EuroMPI/USA 2017, HotInterconnect 25, CARLA 2017, and of the Exacomm ISC workshop and COLOC Euro-Par workshop.
- Guillaume AUPY was a member of the program committee of ICPP’17, SC’17, FTS’17.
- Alexandre DENIS was a member of the program committee of CCGrid 2017, HiPC 2017, Com-Pas’2017, CCGrid 2018.
- Guillaume AUPY was a member of the program committee of EuroMPI/USA 2017, HPCS 2017 and CCGrid 2018.

10.1.2.5. Reviewer
- Alexandre DENIS was a reviewer for Cluster 2017.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards
- Guillaume AUPY was an invited editor for the Special Issue of Concurrency and Computation: Practice and Experience on data structures and algorithms.
- Emmanuel JEANNOT is associate editor of the International Journal of Parallel, Emergent & Distributed Systems (IJPEDS).

10.1.3.2. Reviewer - Reviewing Activities
- Alexandre DENIS was a reviewer for TPDS and JPDC.
- Guillaume AUPY was a reviewer for TPDS and Optimization Methods and Software.
- Emmanuel JEANNOT was reviewer for TPDS, IJHPCA.
10.1.4. Invited Talks

- Brice GOGLIN gave a talk about the structural modeling of next-generation memory architectures at the Fourth Workshop on Programming Abstractions for Data Locality (PADAL’17).
- Guillaume AUPY was invited to talk about I/O scheduling in Argonne National Laboratory.

10.1.5. Leadership within the Scientific Community

- Emmanuel JEANNOT, Brice GOGLIN and Pete BECKMAN organized a Birds-of-a-Feather session about *Cross-Layer Allocation and Management of Hardware Resources in Shared Memory Node*. It gathered about 30 people working on various runtime systems, operating systems and applications in the HPC to discuss how to have all these software components collaborate when spawning jobs on hardware resources.
- Guillaume MERCIER is the chairman of the Hardware Topologies Management Working Group of the MPI Forum. This working group was created officially in December by Inria’s impulse and has been rallied since by many institutions taking part in the MPI Forum. The goal of this working group is to standardize hardware topologies management mechanisms and abstractions in the MPI standard.
- Cédric LACHAT organized the first “PaMPA day” meeting 0, at Inria Bordeaux, gathering authors of prominent remeshing software.

10.1.6. Scientific Expertise

- Emmanuel JEANNOT is member of the hiring committee for the junior chair of the I-Site E2S of the university of Pau.
- François PELLEGRINI is member of the foresight committee on scientific and technological information (IST) of Institut national de recherche agronomique (INRA).
- François PELLEGRINI is member of the pedagogical committee of the Alienor lawyer’s school in Bordeaux.
- François PELLEGRINI was invited by *Organisation Internationale de la Francophonie*, as an international expert on software law and economics, to participate in training sessions for the members of the parliaments of Bénin and Cameroon, regarding the impact of digital technologies on digital sovereignty and national legal systems.
- François PELLEGRINI was heard by the Conseil national du numérique (CNNum), on the European directive on free flow of data.
- François PELLEGRINI was heard by the Conseil régional de Nouvelle-Aquitaine, in the context of the definition of their digital roadmap.
- François PELLEGRINI was invited to the thematic seminar on the *social responsibility of algorithms*, organized by the scientific council of *Institut des sciences de l’information et de leurs interactions* (INS2I) of CNRS.

10.1.7. Standardization Activities

TADAAAM attended the MPI Forum meetings on behalf of Inria (where the MPI standard for communication in parallel applications is developed and maintained). TADAAAM also proposed the creation of a new working group in the MPI Forum, dedicated to hardware topologies management and currently leads this working group. The HSPLIT proposal in currently under early discussions for submission to the forum and eventual inclusion in the MPI standard.

10.1.8. Research Administration

Emmanuel JEANNOT is member of the scientific committee of the Labex IRMIA (Université de Strasbourg).

0https://project.inria.fr/pampa/pampa-day/
Emmanuel JEANNOT is the head of the young researcher commission of Inria Bordeaux Sud-Ouest in charge of supervising the hiring of the PhDs and post-doc of the center.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Members of the TADAAM project gave hundreds of hours of teaching at Université de Bordeaux and the Bordeaux INP engineering school, covering a wide range of topics from basic use of computers, introduction to algorithmics and C programming to advanced topics such as probabilities and statistics, computer architecture, operating systems, parallel programming and high-performance runtime systems, as well as software law and personal data.

Brice GOGLIN participated in the building of the section about fundamentals of computer science in the MOOC Informatique et Création Numérique which focuses at bringing basics about computer science to high-school teachers.

10.2.2. Supervision


PhD in progress: Hugo Taboada, communication progression in runtime systems, started in 2015. Advisor: Alexandre Denis and Emmanuel Jeannot.


10.2.3. Juries

Guillaume MERCIER was a member of the Ph.D defense jury of Fernando Mendonca (supervisor: Denis Trystram, Professor at Grenoble Institute of Technology).

Emmanuel JEANNOT was member of the Ph.D defense jury of:
- Christopher Haine (University of Bordeaux, President)
- Pedro De Souza Bento Da Silva (University of Lyon, ENS Lyon, Reviewer)

Emmanuel JEANNOT was reviewer of the habilitation thesis of Luiz-Angelo Steffenel (University of Reims)

François PELLEGRINI was reviewer and member of the Ph.D defense jury of Thomas Gonçalves (University of Grenoble-Alpes / CEA. Supervisors: Frédéric Desprez, Jean-François Méhaut and Marc Perache).

10.3. Popularization

10.3.1. Duties

Guillaume AUPY was in charge of hosting the undergraduate students (L3) from ENS Lyon and later ENS Cachan at Inria Bordeaux-Sud Ouest.
Brice GOGLIN is in charge of the diffusion of the scientific culture for the Inria Research Centre of Bordeaux. He organized several popularization activities involving colleagues. Brice GOGLIN was a member of the CGenial contest for science projects in high schools. François PELLEGRINI is vice-president of université de Bordeaux, in charge of digital issues.

10.3.2. Online Content
François PELLEGRINI wrote a tribune in the Binaire blog run by Inria staff and hosted by Le Monde, on the “loyalty of data processing”. See: http://binaire.blog.lemonde.fr/2017/03/27/les-algos-ni-loyaux-ni-ethiques/ .

10.3.3. Teaching and Education
- Brice GOGLIN was involved in the MOOC Informatique et Création Numérique which focuses at bringing basics about computer science to high-school teachers. After recording videos, he answered numerous questions on the forum, and during a live hangout about computer architectures and networks. More than 12 000 people registered to the course, and more than 1 200 successfully finished it.
- Brice GOGLIN presented tools for teaching basics of computer science in classes at the teachers’ forum at Cap Sciences.
- François PELLEGRINI participated in the creation of video contents for the MOOC Innov+, on the economics of innovation, published on the FUN platform. His contribution concerns the software economy and law. See: https://www.fun-mooc.fr/courses/course-v1:ubordeaux+28002+session01/about .
- François PELLEGRINI was offered the chair on digital issues at Université populaire de Bordeaux, and gave four lectures on: “The digital revolution”, “Liberties in the digital age”, “Personal data and big data”, “Software law and libre software”. See: http://www.upbordeaux.fr/Le-numerique .

10.3.4. Talks and Hands-on
- Guillaume AUPY presented problems revolving around High-Performance Computing to High-School students during Fête de la Science.
- Guillaume AUPY gave a talk at the seminar Convergence des Droits et du Numérique about differences and common grounds between mathematical logics and juridic logics.
- Brice GOGLIN gave several talks about computer architecture, high performance computing, and research careers to general public audience, school students. He also gave several hands-on sessions about basics of algorithmics and computer science.
- François PELLEGRINI gave many talks on liberties in the digital world, digital sovereignty, software law and economy, artificial intelligence for legal practice, etc., in front of various audiences: Cap Sciences, ESI Brussels, Lycée Borda in Pau, FACTS festival on arts & sciences in Bordeaux, Cinéma Utopia, CURIE congress in Marseille, Observatoire de Nice, the Defense Security Cyber summer school in Bordeaux, the Réseau Cepage of CNRS Aquitaine, etc.

10.3.5. Popularizing inside Inria
Guillaume AUPY presented problems revolving around High-Performance Computing during the seminar Unithé ou Café.

11. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journal


Invited Conferences
International Conferences with Proceedings

[12] F. Pellegrini. À la recherche de la souveraineté numérique, in “École d’été Defense Security Cyber”, Bordeaux, France, Forum Montesquieu, université de Bordeaux and IdEx de l’université de Bordeaux, June 2017, https://hal.inria.fr/hal-01550358.

International Conferences with Proceedings


[22] B. Goglin. On the Overhead of Topology Discovery for Locality-aware Scheduling in HPC, in "PDP2017 - 25th Euromicro International Conference on Parallel, Distributed and Network-Based Processing", St Petersburg, Russia, Proceedings of the 25th Euromicro International Conference on Par-


National Conferences with Proceeding


Conferences without Proceedings


Books or Proceedings Editing


Research Reports


[34] G. Aupy, Y. Robert, F. Vivien. *Assuming failure independence: are we right to be wrong?*, Inria, July 2017, n° RR-9078, https://hal.inria.fr/hal-01556292.


[37] E. Jeannot, F. Mansouri, G. Mercier. *A Hierarchical Model to Manage Hardware Topology in MPI Applications*, Inria Bordeaux Sud-Ouest ; Bordeaux INP ; LaBRI - Laboratoire Bordelais de Recherche en Informatique, June 2017, n° RR-9077, 23, https://hal.inria.fr/hal-01538002.


**Other Publications**


References in notes