Activity Report 2011

Section New Results

Edition: 2012-03-22
| 1. ALEA Project-Team                        | 4 |
| 2. ANUBIS Project-Team                     | 9 |
| 3. BACCHUS Team                            | 11|
| 4. CAGIRE Team                             | 17|
| 5. CARMEN Team                             | 18|
| 6. CEPAGE Project-Team                     | 19|
| 7. CONCHA Project-Team                     | 26|
| 8. CQFD Project-Team                       | 35|
| 9. FLOWERS Project-Team                    | 43|
| 10. GEOSTAT Project-Team                   | 51|
| 11. HIEPACS Project-Team                   | 55|
| 12. IPARLA Project-Team                    | 59|
| 13. LFANT Project-Team                     | 64|
| 14. MAGIQUE-3D Project-Team                 | 67|
| 15. MAGNOME Project-Team                   | 75|
| 16. MC2 Project-Team                       | 79|
| 17. PHOENIX Project-Team                   | 83|
| 18. REALOPT Project-Team                   | 85|
| 19. RUNTIME Project-Team                   | 92|
5. New Results

5.1. Snell envelope with small probability criteria

We present in [33] a new algorithm to compute the Snell envelope in the specific case where the criteria to optimize is associated with a small probability or a rare event. This new approach combines the Stochastic Mesh approach of Broadie and Glasserman with a particle approximation scheme based on a specific change of measure designed to concentrate the computational effort in regions pointed out by the criteria. The theoretical analysis of this new algorithm provides non asymptotic convergence estimates. Finally, the numerical tests confirm the practical interest of this approach.

5.2. On the concentration properties of Interacting particle processes

In [34], we present some new concentration inequalities for Feynman-Kac particle processes. We analyze different types of stochastic particle models, including particle profile occupation measures, genealogical tree based evolution models, particle free energies, as well as backward Markov chain particle models. We illustrate these results with a series of topics related to computational physics and biology, stochastic optimization, signal processing and bayesian statistics, and many other probabilistic machine learning algorithms. Special emphasis is given to the stochastic modeling and the quantitative performance analysis of a series of advanced Monte Carlo methods, including particle filters, genetic type island models, Markov bridge models, interacting particle Markov chain Monte Carlo methodologies.

5.3. A Robbins-Monro procedure for estimation in semiparametric regression models

The paper [39] is devoted to the parametric estimation of a shift together with the nonparametric estimation of a regression function in a semiparametric regression model. We implement a Robbins-Monro procedure very efficient and easy to handle. On the one hand, we propose a stochastic algorithm similar to that of Robbins-Monro in order to estimate the shift parameter. A preliminary evaluation of the regression function is not necessary for estimating the shift parameter. On the other hand, we make use of a recursive Nadaraya-Watson estimator for the estimation of the regression function. This kernel estimator takes in account the previous estimation of the shift parameter. We establish the almost sure convergence for both Robbins-Monro and Nadaraya-Watson estimators. The asymptotic normality of our estimates is also provided.

5.4. Discrete Time Markovian Agents Interacting Through a Potential

A discrete time stochastic model for a multiagent system given in terms of a large collection of interacting Markov chains is studied. The evolution of the interacting particles is described through a time inhomogeneous transition probability kernel that depends on the ’gradient’ of the potential field. The particles, in turn, dynamically modify the potential field through their cumulative input. Interacting Markov processes of the above form have been suggested as models for active biological transport in response to external stimulus such as a chemical gradient. One of the basic mathematical challenges is to develop a general theory of stability for such interacting Markovian systems and for the corresponding nonlinear Markov processes that arise in the large agent limit. Such a theory would be key to a mathematical understanding of the interactive structure formation that results from the complex feedback between the agents and the potential field. It will also be a crucial ingredient in developing simulation schemes that are faithful to the underlying model over long periods of time. The goal of the work developed in [42] is to study qualitative properties of the above stochastic system as the number of particles (N) and the time parameter (n) approach infinity. In this regard asymptotic properties of a deterministic nonlinear dynamical system, that arises in the propagation of chaos...
limit of the stochastic model, play a key role. We show that under suitable conditions this dynamical system has a unique fixed point. This result allows us to study stability properties of the underlying stochastic model. We show that as $N \to \infty$, the stochastic system is well approximated by the dynamical system, uniformly over time. As a consequence, for an arbitrarily initialized system, as $N \to \infty$ and $n \to \infty$, the potential field and the empirical measure of the interacting particles are shown to converge to the unique fixed point of the dynamical system. In general, simulation of such interacting Markovian systems is a computationally daunting task. We propose a particle based approximation for the dynamic potential field which allows for a numerically tractable simulation scheme. It is shown that this simulation scheme well approximates the true physical system, uniformly over an infinite time horizon.

5.5. An Adaptive Interacting Wang-Landau Algorithm for Automatic Density Exploration

While statisticians are well-accustomed to performing exploratory analysis in the modeling stage of an analysis, the notion of conducting preliminary general-purpose exploratory analysis in the Monte Carlo stage (or more generally, the model-fitting stage) of an analysis is an area which we feel deserves much further attention. Towards this aim, the paper [41] proposes a general-purpose algorithm for automatic density exploration. The proposed exploration algorithm combines and expands upon components from various adaptive Markov chain Monte Carlo methods, with the Wang-Landau algorithm at its heart. Additionally, the algorithm is run on interacting parallel chains – a feature which both decreases computational cost as well as stabilizes the algorithm, improving its ability to explore the density. Performance is studied in several applications. Through a Bayesian variable selection example, the authors demonstrate the convergence gains obtained with interacting chains. The ability of the algorithm’s adaptive proposal to induce mode-jumping is illustrated through a trimodal density and a Bayesian mixture modeling application. Lastly, through a 2D Ising model, the authors demonstrate the ability of the algorithm to overcome the high correlations encountered in spatial models.

5.6. A sharp analysis on the asymptotic behavior of the Durbin-Watson statistic for the first-order autoregressive process

The purpose of the paper [40] is to provide a sharp analysis on the asymptotic behavior of the Durbin-Watson statistic. We focus our attention on the first-order autoregressive process where the driven noise is also given by a first-order autoregressive process. We establish the almost sure convergence and the asymptotic normality for both the least squares estimator of the unknown parameter of the autoregressive process as well as for the serial correlation estimator associated to the driven noise. In addition, the almost sure rates of convergence of our estimates are also provided. It allows us to establish the almost sure convergence and the asymptotic normality for the Durbin-Watson statistic. Finally, we propose a new bilateral statistical test for residual autocorrelation.

5.7. Large deviations for Gaussian stationary processes and semi-classical analysis

In [37], we obtain a large deviation principle for quadratic forms of Gaussian stationary processes. It is established by the conjunction of a result of Roch and Silbermann on the spectrum of products of Toeplitz matrices together with the analysis of large deviations carried out by Gamboa, Rouault and the rst author. An alternative proof of the needed result on Toeplitz matrices, based on semi-classical analysis, is also provided.

5.8. Sharp large deviations for the non-stationary Ornstein-Uhlenbeck process

For the Ornstein-Uhlenbeck process, the asymptotic behavior of the maximum likelihood estimator of the drift parameter is totally different in the stable, unstable, and explosive cases. Notwithstanding of this trichotomy, we investigate sharp large deviation principles for this estimator in the three situations. In the explosive case, we exhibit in [38] a very unusual rate function with a shaped flat valley and an abrupt discontinuity point at its minimum.
5.9. Markovian quadratic and superquadratic BSDEs with an unbounded terminal condition

The work in [43] deals with the existence and the uniqueness of solutions to quadratic and superquadratic Markovian backward stochastic differential equations (BSDEs for short) with an unbounded terminal condition. Our results are deeply linked with a strong a priori estimate on $Z$ that takes advantage of the Markovian framework. This estimate allows us to prove the existence of a viscosity solution to a semilinear parabolic partial differential equation with nonlinearity having quadratic or superquadratic growth in the gradient of the solution. This estimate also allows us to give explicit convergence rates for time approximation of quadratic or superquadratic Markovian BSDEs.

5.10. New approach on recursive and non-recursive SIR

In [3], we consider a semiparametric single index regression model involving a p-dimensional quantitative covariable $x$ and a real dependent variable $y$. A dimension reduction is included in this model via an index $x^T \beta$. Sliced inverse regression (SIR) is a well-known method to estimate the direction of the Euclidean parameter $\beta$ which is based on a "slicing step" of $y$ in the population and sample versions. The goal of this paper is twofold. On the one hand, we focus on a recursive version of SIR which is also suitable for multiple indices model. On the other hand, we propose a new method called SIRoneslice when the regression model is a single index model. The SIRoneslice estimator of the direction of $\beta$ is based on the use of only one "optimal" slice chosen among the H slices. Then, we provide its recursive version. We give an asymptotic result for the SIRoneslice approach. Simulation study shows good numerical performances of the SIRoneslice method and clearly exhibits the main advantage of using recursive versions of the SIR and SIRoneslice methods from a computational time point of view. A real dataset is also used to illustrate the approach. The proposed methods and criterion have been implemented in R and the corresponding codes are made available.

5.11. Classification of EEG data by evolutionary algorithm for the study of vigilance states

The objective of this work [18] is to predict the state of vigilance of an individual from the study of its brain activity (EEG signals). The variable to predict is binary (alertness "normal" or "relaxed"). EEG of 44 participants in both states (88 records) were collected with a helmet with 58 electrodes. After a pretreatment step and data validation, a test called "test slope" was chosen. The usual methods of supervised classification (k nearest neighbors, binary classification trees, random forests, and discriminant sparse PLS) were used to provide predictions of the state of participants. The test was then refined using a genetic algorithm, which has built a reliable model (average true classification rate by using CART equal to 86.68 +/- 1.87%) and to select an electrode from the initial 58.

5.12. Genetic Programming

Recently, it has been stated that the complexity of a solution is a good indicator of the amount of overfitting it incurs. However, measuring the complexity of a program, in Genetic Programming, is not a trivial task. In [22], we study the functional complexity and how it relates with overfitting on symbolic regression problems. We consider two measures of complexity, Slope-based Functional Complexity, inspired by the concept of curvature, and Regularity-based Functional Complexity based on the concept of Holderian regularity. In general, both complexity measures appear to be poor indicators of program overfitting. However, results suggest that Regularity-based Functional Complexity could provide a good indication of overfitting in extreme cases.

During the development of applied systems, an important problem that must be addressed is that of choosing the correct tools for a given domain or scenario. This general task has been addressed by the genetic programming (GP) community by attempting to determine the intrinsic difficulty that a problem poses for a GP search. In [21], we present an approach to predict the performance of GP applied to data classification, one of the most common problems in computer science. The novelty of the proposal is to extract statistical descriptors
and complexity descriptors of the problem data, and from these estimate the expected performance of a GP classifier. We derive two types of predictive models: linear regression models and symbolic regression models evolved with GP. The experimental results show that both approaches provide good estimates of classifier performance, using synthetic and real-world problems for validation. In conclusion, this paper shows that it is possible to accurately predict the expected performance of a GP classifier using a set of descriptors that characterize the problem data.

The analysis of image regularity using Holder exponents can be used to characterize singular structures contained within an image, and provide a compact description of local shape and appearance. However, estimating the Holder exponent is not a trivial task and current methods tend to be slow and complex. Therefore, the goal in [35] is to automatically synthesize image operators that can be used to estimate the Holder regularity of an image. We pose this task as an optimization problem and use Genetic Programming (GP) to search for operators that can approximate a traditional estimator, the oscillations method. In our experiments, GP was able to evolve estimators that achieve a low error and a high correlation with the ground truth estimation. Furthermore, most of the GP estimators are faster than the traditional approaches, in some cases their runtime is orders of magnitude smaller. This result allowed us to implement a real-time estimation of the Holder exponent on a live video signal, the first such implementation in current literature. Moreover, the evolved estimators are used to generate local descriptors of salient image regions, a task for which we obtain a stable and robust matching that is comparable with state-of-the-art methods. In conclusion, the evolved estimators produced by GP could help expand the application domain of Holderian regularity within the fields of image analysis and signal processing.

5.13. Relevance of the Holderian regularity-based interpolation for range-Doppler ISAR image post-processing

In ISAR processing, post-processing of the range Doppler image is useful to help the practitioner for ship recognition. Among the image post-processing tools, interpolation methods can be of interest especially when zooming. In [19], we study the relevance of the Holderian regularity-based interpolation. In that case, interpolating consists in adding a new scale in the wavelet transform and the new wavelet coefficients can be estimated from others. In the original method, initially proposed by two of the authors, the image is first interpolated along the rows and then along the columns. Concerning the diagonal pixels, they are estimated as the mean of the adjacent original and interpolated pixels. Here, we propose a variant where the diagonal pixels are estimated by taking into account the local orientation of the image. It has the advantage of conserving local regularity on all interpolated pixels of the image. A comparative study on synthetic data and real range-Doppler images is then carried out with alternative interpolation techniques such as the linear interpolation, the bicubic one, the nearest neighbour interpolation, etc. The simulation results confirm the effectiveness of the approach.

5.14. On-line changepoint detection and parameter estimation with application to genomic data

We propose in [10] an efficient on-line changepoint detection algorithm for an important class of Bayesian product partition models. The algorithm allows to estimate jointly on-line the static parameters of the model using a recursive maximum likelihood estimation strategy. This particle filter type algorithm has a computational complexity which scales linearly both in the number of data and the number of particles. We demonstrate our methodology on a synthetic and two real world datasets from RNA transcript analysis. On simulated data, it is shown that our approach outperforms standard techniques used in this context and hence has the potential to detect novel RNA transcripts.

5.15. Bayesian Sparsity-Path-Analysis of Genetic Association Signal using Generalized t Priors
In [17], we explore the use of generalized t priors on regression coefficients to help understand the nature of association signal within "hit regions" of genome-wide association studies. The particular generalized t distribution we adopt is a Student distribution on the absolute value of its argument. For low degrees of freedom we show that the generalized t exhibits 'sparsity-prior' properties with some attractive features over other common forms of sparse priors and includes the well known double-exponential distribution as the degrees of freedom tends to infinity. We pay particular attention to graphical representations of posterior statistics obtained from sparsity-path-analysis (SPA) where we sweep over the setting of the scale (shrinkage / precision) parameter in the prior to explore the space of posterior models obtained over a range of complexities, from very sparse models with all coefficient distributions heavily concentrated around zero, to models with diffuse priors and coefficients distributed around their maximum likelihood estimates. The SPA plots are akin to LASSO plots of maximum a posteriori (MAP) estimates but they characterize the complete marginal posterior distributions of the coefficients plotted as a function of the precision of the prior. Generating posterior distributions over a range of prior precisions is computationally challenging but naturally amenable to sequential Monte Carlo (SMC) algorithms indexed on the scale parameter. We show how SMC simulation on graphic-processing-units (GPUs) provides very efficient inference for SPA. We also present a scale-mixture representation of the generalized t prior that leads to an EM algorithm to obtain MAP estimates should only these be required.
5. New Results

5.1. New results in the theory of factorization of boundary value problems

Participants: Jacques Henry, Fadhel Jday, Maria Orey.

We are pursuing the development of the theory of factorization of boundary value problems as described in 3.1. Maria Orey who suspended her PhD thesis for a while due to health reason, has resumed her work on extending the method of factorization to the analogous in infinite dimension of the QR algorithm for matrices. This passes through the factorization of the normal equation for the least squares problem. This problem is solved and this allows a clear definition of the Q and R operators. She will defend her thesis in 2012.

F. Jday has obtained also a clear formulation for the factorization of the Stokes equation.

A progress has been made in the attempt to extend the factorization method to parabolic evolution equation. It appears that it is not the evolution problem that can be factorized with respect to space but the evolution operator \( S(t) \) that transfers the solution from time 0 to \( t \). The corresponding Riccati equation has been obtained but a full mathematical justification remains to be done.

5.2. Data completion problems for elliptic equations using the theory of factorization

Participants: Jacques Henry, Fadhel Jday.

F. Jday is continuing his thesis co-supervised by A. Ben Abda and J. Henry. The use of the method of factorization for the data completion problem has been presented in a paper in Inverse Problems when the domain is a cylinder, both Dirichlet and Neumann data are known on one face and are to be estimated on the other. Dirichlet boundary conditions were assumed on the lateral boundary. In relation to the inverse problem in electrocardiology one has to take into account more complex geometries. F. Jday considered the domain limited by two concentric spheres. The method still applies considering the family of concentric spheres deduced by homothety.

5.3. Modeling the activity of populations of neurons: study of synchronization

Participants: Jacques Henry, Gregory Dumont, Oana Tarniceriu.

During the second year of his PhD thesis G. Dumont continued to develop and refine a simulator of a population of leaky integrate and fire neurons, with a finite jump of potential response to a synaptic stimulation in order to compare with the results from another approach, the Fokker-Planck approach. It would be interesting to show that the Fokker Planck approach can be seen as a limiting case, for high frequency small jump of potential, of the one of B. Knight, L. Sirovich and L. Omurtag. At least it is suggested by the simulations. The second year focused on the study of mathematical aspects of the equation. The methods were inspired by the book of Benoit Perthame: Transport equation in biology. With these tools, the mathematical properties of the model of population density have been established: the existence and uniqueness of a solution. G. Dumont has also been able to establish that in special cases the equation has no solution, or more precisely that the solution blows up, assuming that there is no conduction delay of the spikes within the considered population. This blow up can be related to a synchronization. In case of a conduction delay the condition of existence of a solution are much larger. The situation of inhibiting synapses has also been studied. This has been submitted to the Journal of Mathematical Biosciences.

Using the principles of entropy, G. Dumont has shown that under certain circumstances the solution of the equation converges to a stationary solution and this can be interpreted as the desynchronization of the population of neurons.
Similar studies have been done on the thetaneuron model which accounts for self spiking neurons. The question of the synchronization of a population of neurons is also studied in collaboration with O. Tarniceriu. We consider a population of identical self firing neurons that are weakly coupled and we study the long term evolution of the reapportion of phases. We are now focusing to a population of 1D leaky integrate and fire neurons and we expect more precise results for this simple model.

5.4. Modeling in electrocardiology

Participants: Bedr’Eddine Ainseba, Jacques Henry, Yves Coudière, Simon Labarthe, Alejandro Lopez Rincon.

5.4.1. Modeling the electrical activity of the atria

The first year of the PhD thesis of Simon Labarthe has been dedicated to three main activities:

- a review of medical and mathematical literature about anatomy and physiology of atria and atrial fibrillation, numerical simulation of cardiac activity, mathematical analysis of cardiac models.
- the numerical implementation of simulation tools has been developed: the software is able to take into account a real 3D or 2D manifold geometry with realistic fibre orientation to simulate the bidomain or monodomain problem. Geometrical tools facilitating the fibre orientation construction have been added.
- numerical and theoretical studies of the modeling and the influence of fibre orientation in the atria and the pulmonary veins have been initiated.

5.4.2. Inverse problem in electrocardiology

The PhD thesis of Alejandro Lopez is devoted to improving the resolution of the inverse problem to recover the potential map on the heart from the measured potentials on the torso.

To have a best solution of the inverse problem many steps were taken. First, a software to solve the finite element method in 3d for the Poisson equation was created, and compared to an analytical solution. Also a software for the heat equation was created to prepare the monodomain equation. The improvement of the forward solution helps to improve the inverse solution. An article explaining the software was included in the book "VEHÍCULOS AEROESPACIALES" (aerospace vehicles) published by the Sociedad Mexicana de Ciencia y Tecnología Aeroespacial (Mexican Society of Aerospace Science, and Technology) [19].

The second step was to develop a static solution of the inverse problem constructing a transfer matrix (heart to thorax), and solving with conjugate gradient. An article describing this software was accepted in the 22nd International Conference on Electronics, Communications and Computers.

As a third step the boundary element method was implemented to see the advantages and disadvantages in comparison with the finite element method.

The next step was to implement the monodomain model of the heart, to try to solve the problem of identification of parameters (in progress).

5.5. Invasion processes and modeling in epidemiology

Participants: Jean-Baptiste Burie, Arnaud Ducrot.

We have derived a homogenized version of our model of a fungal of disease of vine(see [7]) that takes into account the periodic row structure of vineyards. We used two-scale homogenization of Nguentseng and Allaire (see e.g. [20]): the macroscopic scale is the vineyard scale while the microscopic one is the plant scale. We have proved a result of convergence towards the homogenized model and numerical simulations have demonstrated a significant gain in computing time and stability.

These results have been presented at ECMTB2011 in Krakow (and also, at the Exploratory Workshop on Emerging Infectious Diseases and Mathematical Modelling, Barcelona 2011 and seminars at Franche-Comté University, Tamkang and National Taiwan University).

An article is to be submitted in SIAM J. Multiscale Modeling and Simulation in early 2012.
6. New Results

6.1. Numerical schemes and algorithms for fluid mechanics.

Participants: Rémi Abgrall [Corresponding member], Guillaume Baurin, Pietro Marco Congedo, Cécile Dobrzynski, Marc Duruflé, Dante De Santis, Algiane Froehly, Gianluca Geraci, Robin Huart, Arnaud Krust, Cédric Lachat, Mario Ricchiuto, Birte Schmidtman, Héloïse Beaugendre, Sébastien Blaise.

6.1.1. Residual distribution schemes

This year, many developments have been conducted and implemented in the RealfluiDS and SLOWSSoftware after the initial ideas discussed in [55] and in [64], [61], [65], which have opened up many doors.

First of all, the parallel three dimensional high order extension of the scheme of [55] has been finally validated on several external aerodynamics configurations[3], including the classical ONERA M6 wing case on a large mesh containing $5.5 \times 10^6$ vertices (simulation run on 256 processors), and a business jet configuration in supersonic conditions, on a mesh obtained by the GAMMA3 EPI.

Meanwhile, the improvement of the treatment of viscous terms has been investigated within the PhD theses of G. Baurin and D. DeSantis [46], [19]. The validation on laminar flows of a classical formulation based on a Petrov-Galerkin approach [60], [17] has shown its limitations. An improved formulation, based on a recovery of the solution gradient, has been proposed and tested. In both the second and third order cases, while showing the improvement in accuracy for steady state laminar flows, the results also show a slow iterative convergence, and a systematic small accuracy drop when the cell Reynolds number is of order one. These issues are currently under investigations, while the current formulation is being enhanced by adding a Spalart Almaras turbulent model. Contributions to these activities come from the PhD of Guillaume Baurin, who has implemented the third order version of our methods in a real industrial platform (N3S Natur of SAFRAN developped by Incka), and from the PhD of Dante DeSantis who is developing the turbulent implementation in RealfluiDS within the EU project IDIHOM.

Meanwhile, we are refining and validating the extension of the schemes to elements using improved approximations based on Bézier and NURBS polynomials. The initial two-dimensional implementation [56], [59] of third and fourth order schemes on curved meshes is now being enhanced by adding a local mesh refinement procedure and is also currently being extended to three space dimensions. Contributions to this topic come from the PhD of Algiane Froehly.

R. Abgrall has extended the RDS formalism to Lagrangian hydrodynamics. The results are comparable to what can be obtained for more standard methods, a publication is in preparation.

Concerning time dependent flows, the ideas of [61], [64] have led to two main lines of developments. On one hand, the unconditionally second order and stable space-time approach of [61] has been further validated [14] and extended to higher orders of accuracy [51]. The main advantage of this technique is its ability to preserve monotonicity unconditionally w.r.t. the time step. This has interesting applications in shallow water flows [36] in which the schemes previously developed [65] did allow to preserve the positivity of the water depth, however with an inefficient implicit procedure constrained by an explicit-type time step restriction.

In parallel, the genuinely explicit formulation of [64] has been combined with the positivity preserving approach of [65] to obtain a genuinely explicit positivity preserving scheme for shallow water simulations [16]. With a time step restriction quite close to that necessary for the scheme of [65], the approach proposed allows a very efficient explicit time stepping with a tenfold reduction of the computational time for the same accuracy level.
These developments are implemented in the SLOWS platform and are thoroughly summarized in the manuscript [2]. We now dispose of a spectrum of numerical tools allowing either classical temporal integration based on implicit multistep schemes, or on unconditionally stable and positivity preserving space-time schemes, or on a genuinely explicit approach. Current developments aim at extending these tools to arbitrary accuracy, and at developing hybrid implicit/explicit approaches.


In this work, Héloïse Beaugendre, Boniface Nkonga and Christelle Wervaecke proposed a strongly coupled numerical formulation for the Spalart-Allmaras model, in the framework of Stabilized Finite Element Methods. Computations are performed for compressible Newtonian fluids (2D and 3D) on unstructured grids of high aspect ratio. Results are compared with experimental data and also with solutions obtained by different numerical strategies. The additional transport equations for subscale model are often numerically weakly coupled to Navier-Stokes equations through operator splitting. These variables are strongly coupled for the transport process within a stabilized finite element formulation. The stabilization tensor is defined, such as to reduce mesh dependencies and to still be consistent at the asymptotic of highly anisotropic meshes. Indeed, this tensor involves a measure of the local length scale $h$ which can be difficult to define in the case of a stretched element. In this work, the local length scale is implicitly given by the inverse of the absolute flux Jacobian matrix as proposed in Barth (1998) and more recently in Abgrall (2006). The stabilized finite element strategy is also suitable for complex geometries and the resulting schemes have a compact stencil which we exploit for efficient parallel strategies combining domain decomposition and message passing tools (MPI).

### 6.1.3. Uncertainty quantification

R. Abgrall and P.M. Congedo have made a detailed comparison between the semi-intrusive method developed last year with more classical non intrusive polynomial chaos methods, and Monte Carlo results. The effectiveness of this method is illustrated for a modified version of Kraichnan-Orszag three-mode problem where a discontinuous pdf is associated to the stochastic variable, and for a nozzle flow with shocks. The results have been analyzed in terms of accuracy and probability measure flexibility. Finally, the importance of the probabilistic reconstruction in the stochastic space is shown up on an example where the exact solution is computable, the viscous Burgers equation. These results have been reported in [25], [47].

Following this studies, two contributions have been obtained within the context of Gianluca Geraci’s thesis. First one is an adaptive strategy, inspired by the Harten multi-resolution framework that has been developed in order to compute efficiently statistics. This preliminary work aims to show the potentialities of this approach in order to evaluate the possibility to include this strategy in the semi-intrusive method developed in the recent years. We obtained [34] well-converged results with a lower computational cost due to a reduction of the numerical evaluations.

Second contribution [48] is a study concerning the Sparse Grid techniques coupled with Polynomial Chaos for multi-dimensional stochastic problems. Sparse grid techniques have been used to compute the multi-dimensional integrals needed to evaluate the coefficients of the polynomial expansion. We also investigated the possibility to reduce the number of random variables by means of an ANOVA analysis.

P.M. Congedo investigated the possibility to perform a stochastic inverse analysis by using an hybrid method within a Polynomial Chaos/Genetic Algorithms framework. This strategy has been applied on the numerical simulation of a dense gas shock-tube. Previous theoretical and numerical studies have shown that a rarefaction shock wave (RSW) is relatively weak and that the prediction of its occurrence and intensity are highly sensitive to uncertainties on the initial flow conditions and on the fluid thermodynamic model. The objective of this work has been to introduce an innovative, flexible and efficient algorithm combining computational fluid dynamics (CFD), uncertainty quantification (UQ) tools and metamodel-based optimization in order to obtain a reliable estimate for the RSW probability of occurrence and to prescribe the experimental accuracy requirements ensuring the reproducibility of the measurements with sufficient confidence.

Uncertainty quantification tools have been used to perform some applicative studies on epistemic uncertainties, in particular on some complex equations of state [8], and some turbulence [12] models. We have also started
considering the influence of model parameters uncertainties in free surface models for long-waves such as
 tsunamis [52], coupling the numerics developed in the team for shallow-water flows [53] and the tools
 available for uncertainty quantifications. This is certainly a field of application where these developments will
demonstrate very useful.

Within the associated team AQUARIUS activities (collaboration with Stanford University), two efficient
 global strategy for robust optimization have been developed. First one is based on the extension of simplex
 stochastic collocation to the optimization space, while the second one consists in an hybrid strategy using
 ANOVA decomposition. The Simplex Stochastic Collocation (SSC) method has been developed for adaptive
 uncertainty quantification (UQ) in computational problems with random inputs. In this work [30], we showed
 how this formulation based on Simplex space representation, discretization of non-hypercube probability
 spaces and adaptive refinements can be easily coupled with a well-known optimization method, i.e. Nelder-
 Mead algorithm, also known as Downhill Simplex Method. Numerical results showed that this method is very
efficient for mono-objective optimization and minimizes global number of deterministic evaluations in order
to determine optimal design. This method has been then applied to a realistic problem of robust optimization
of a two-component race-car airfoil.

We proposed also an efficient strategy [29] for robust optimization when a large number of uncertainties is
taken into account. ANOVA analysis is used in order to perform a variance-based decomposition and to reduce
stochastic dimension. A massive use of metamodels allows reconstructing response surfaces for sensitivity
indexes and fitness function in the design variables plan. Proposed strategy has been applied to the robust
optimization of a turbine cascade for thermodynamically complex flows.

6.1.4. Multiphase flows

Starting from [58], R. Abgrall and H. Kumar are developing a methods that is able to compute multiphase
flows when the interfacial area takes any value. In the previous version, either we could take into account
infinite interfacial areas or pure interface problems. M.G. Rodio is developing, along similar lines, a scheme
for the Navier Stokes equations.

6.1.5. Numerical schemes for advanced materials

Two parallel lines of work on developments of numerical models for advanced materials have seen important
developments this year.

On one hand, Rémi Abgrall and Pierre-Henri Maire (CEA Cesta) are extending the Lagrangian method
developed a couple years ago and currently implemented in the CHIC code to elastodynamics. The stress
tensor is no longer diagonal and here we consider the Wilkins model. The main difficulty is to understand the
role of the second principle and how to deal with the von Mises criteria.

In parallel, Mario Ricchiuto and the group led by Gérard Vignoles at LCTS (UMR-5801 LCTS) have been
developing a finite element numerical model of the evolution of the liquid oxide evolution during the healing-
phase taking place in the silicon-based composite materials similar to those used in SAFRAN’s new aero-
engines 1 [50]. This micro-model is meant to be used as a numerical closure for the LCTS’ structural
mechanics solver [31], allowing to obtain a faithful description of the material’s behavior, including the
effects of the healing process.

6.1.6. Discontinuous Galerkin schemes, New elements in DG schemes

Rémi Abgrall and Pierre-Henri Maire (CEA CESTA), with François Vilar (PhD at CELIA funded by a CEA
grant started in October 2009), are working on fully Lagrangian schemes within the Discontinuous Galerkin
schemes. The idea is to start from the formulation of the Euler equation in full Lagrange coordinates: the spatial
derivative are written in Lagrangian coordinates. The mesh element are now curved and we are working on
the geometrical conservation law. The application to several standard test case indicate the potential of the
method.

6.1.7. Penalization techniques with unstructured adapted meshes

Penalization methods are an efficient alternative to explicitly impose boundary conditions but their accuracy is generally of first order. In this work we combine the easiness of penalization techniques with the precision of unstructured anisotropic mesh adaptation. Level sets are used to describe the geometry so that geometrical and topological changes due to physics are straightforward to follow. Navier-Stokes simulations are performed and a new way to impose a slipping wall boundary condition is proposed.

6.1.8. Mesh adaptation

A work on high order mesh generation has been pushed further. Starting with a $P^1$ (triangle) mesh and some information on the boundary (control point), we are able to generate a valid third order curved mesh. The algorithm is based on edge swaps and is similar to a boundary enforcement procedures. This method is very robust but not efficient of the boundary layer. Indeed the edge swaps destroy a part of the boundary layer. To solve this problem, we investigate the use of linear elasticity to curve a $P^1$ mesh.

Moreover, we started to make high order mesh adaptation. That means we are able to refine high order meshes where the error is maximum and so we generate non uniform meshes of order $k$ with $k > 2$. We compute Euler compressible simulations on those meshes to validate the mesh adaptation strategy.

In parallel to these developments, we have started work on a generalized formal approach to obtain discrete adjoint equations for residual based and Petrov-Galerkin finite element schemes [49]. We have shown that these discrete adjoint equations can now be used as a local error estimator for mesh refinement, giving to these methods to the same potential for adaptation of Galerkin schemes.

6.2. High performance simulation for plasma physics

Participants: Rémi Abgrall, Robin Huart, Xavier Lacoste, François Pellegrini, Pierre Ramet [Corresponding member].

In the RealfluïDS code, the Rusanov scheme for Ideal MHD has already shown its ability to capture discontinuities and its robustness many times in 2D problems [57]. But other spatial schemes could be interesting for applications in tokamak experiments, since we may not encounter strong shocks in these cases. Hence, according to the type of the problem, coupled schemes could be used. We already developed the 4 well known base RD schemes: Narrow, LDA, Rusanov and SU (a RD version of the SUPG scheme). Coupling may not be challenging, a working shock sensor is already implemented for stabilized methods. Very high order of accuracy (at least 3rd order) should be reachable in all cases, the main parts of this work have already been done for several types of elements. The non-dimensionalized equations of resistive MHD (with viscosity and heat transfer) have been added to the code with a Continuous Galerkin discretization. Also, 2nd order implicit and explicit methods were developed in all cases. Once we succeed in ensuring a very good iterative convergence, taking into account the hyperbolic divergence cleaning technique in an unsteady context, we will be able to simulate plasma instabilities. This is really the key issue for now. These results will be presented in the PhD defense of R. Huart planned at January 2012.

The JOREK code is now able to use several hundred of processors routinely. Simulations of ELMs are produced taking into account the X-point geometry with both closed and open field lines. But a higher toroidal resolution is required for the resolution of the fine scale filaments that form during the ELM instability. The complexity of the tokamak’s geometry and the fine mesh that is required leads to prohibitive memory requirements. In the current release, the memory scaling is not satisfactory: as one increases the number of processes for a given problem size, the memory footprint on each process does not reduce as much as one can expect.

In the context of the new ANR proposal (ANEMOS project), we are working to reduce memory consumers in the JOREK code. Compression techniques can be foreseen to reduce the footprint of the matrix without having to pay large computation expenses. Moreover, the storage of the factorized preconditioning matrix inside the direct solver takes also a large amount of memory. We have defined and developed a general programming interface for sparse linear solvers (http://murge.gforge.inria.fr) for which we also provided some test programs and documentation. Our goal is to normalize the application programming interface of
sparse linear solvers and to provide some very simple ways of doing some fastidious tasks such as parallel matrix assembly for instance. This interface has been validated in Realfluids and JOREK for HIPS and PaStiX. Using this common interface, we are looking for a fair distribution of data over the parallel processes in order to reduce memory consumption. The effective parallelization of this assembly step is one of the main bottlenecks up to now, as far as memory usage is concerned. The GMRES driver is also a large consumer in terms of memory and we plan to consider an up-to-date parallel implementation of this step.

6.3. Algorithms and high-performance solvers

Participants: Astrid Casadei, Cécile Dobryniski, Sébastien Fourestier, Damien Genêt, Hervé Guillard [(Pumas)], Laurent Hascoët [(Tropics)], Cédric Lachat, Xavier Lacoste, François Pellegrini, Pierre Ramet [Corresponding member].

6.3.1. Parallel domain decomposition and sparse matrix reordering

Most of the work carried out within the Scotch project (see section 5.7) has been carried out in the context of the PhD of Sébastien Fourestier.

The first axis concerns dynamic repartitioning and remapping. A new set of sequential routines has been devised, which offers new features: mapping (including plain partitioning) with fixed vertices, remapping, and remapping with fixed vertices. All of the above developments are about to be released in the major release 6.0 of Scotch. The porting of the remapping algorithms in parallel is being carried out, and will be part of release 6.1.

A work carried out in the Joint Laboratory for Petascale Computing (JLPC) between INRIA and UIUC resulted in the inclusion of Scotch as a load balancer in the Charm++ parallel environment. A jointly written conference paper has been submitted on this subject. Another potential use of the remapping features of Scotch concerns multi-phase mapping. Experiments are being carried out at UIUC regarding the use of Scotch as a multi-phase mapper for the OpenAtom scientific code.

6.3.2. Parallel mesh adaptation

This research topic deals with the design of efficient and scalable software tools for parallel dynamic remeshing. This is a joint work with Cécile Dobrzynski, in the context of the PhD of Cédric Lachat, funded by a CORDI-S grant managed by the PUMAS team.

PaMPA (see Section 5.11) is a middleware library dedicated to the management of distributed meshes.

The software development of PaMPA is going on. The internal data structure for representing meshes has been frozen, and developments are in progress. The first developments aimed at proving the efficiency of the planned API for handling distributed meshes. A simple P1 FEM Laplacian solver has been written over PaMPA by the PUMAS team to demonstrate how to iterate over PaMPA entities (elements and nodes) and access values borne by the entities, so as to perform FEM computations. These features are available in version 0.1. which has not yet been diffused to other interested parties. Several new potential users are already willing to try out this version, e.g. ONERA.

PaMPA is already used as the data structure manager for two solvers being developed at INRIA: the Plato solver being developed by the PUMAS team, and the Aerosol new generation fluid dynamics solver being developed in the context of the PhD of Damien Genêt. The interaction with these users allows us to refine the interface to match their needs.

This work now focuses on the core of the PhD of Cédric Lachat: interfacing PaMPA with MMG3D to demonstrate the ability of PaMPA to perform parallel mesh adaptation.
6.3.3. **High-performance direct solvers on multi-platforms**

New supercomputers incorporate many microprocessors which include themselves 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 RUNTIME team, we study optimization strategies to improve the scheduling of communications, threads and I/O. Sparse direct solvers are a basic building block of many numerical simulation algorithms. 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.

In collaboration with the ICL team from the University of Tennessee, and the RUNTIME team from INRIA, we are evaluating the way to replace the scheduling driver of the PaStiX solver by one of the generic frameworks, DAGuE (see http://icl.cs.utk.edu/dague/overview/ or StarPU (see http://runtime.bordeaux.inria.fr/StarPU), to execute the task graph corresponding to a sparse factorization. This work now focuses on the core of the PhD of Xavier Lacoste, the aim is to study and design algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with GPU accelerators. This is a joint work with the MUMPS team and algorithms will have to be adapted in order to exhibit parallelism that can be more suitable for the dynamic scheduling of computational tasks on such heterogeneous architectures.

6.3.4. **Hybrid direct-iterative solver based on a Schur complement approach.**

In HIPS, we propose several algorithmic variants to solve the Schur complement system that can be adapted to the geometry of the problem: typically some strategies are more suitable for systems coming from a 2D problem discretisation and others for a 3D problem; the choice of the method also depends on the numerical difficulty of the problem. We have a parallel version of HIPS that provides full iterative methods as well as hybrid methods that mixes a direct factorization inside the domain and an iterative method in the Schur complement.

Graphs or meshes partitioners are now able to deal with problems that have more than several billion of unknowns. Solving linear systems is clearly the limiting step to reach this challenge in numerical simulations. During her PhD, Astrid Casadei will have to propose solutions to get an efficient algorithmic coupling of direct and iterative methods that allow a powerful management of whole the levels of parallelism. As a preliminary study, we focus on memory issues to build a Schur complement in our direct solver. During factorization step, memory overhead may occur for two reasons. The first one is due to the fan-in approach, that is to say the local storage of non-local contributions. The second overhead is due to the coupling matrices (between direct part and Schur complement), which remain allocated during the whole computation and are freed only at the end. Our first ideas to reduce memory consumption was to postpone the allocation of each block and, thanks to a right-looking algorithm, a column-block may be freed as soon as it has been treated. However, many blocks may be allocated very quickly, and a solution would be to use a left-looking scheme when dealing with local contributions. Thus, we introduce a mixed version : a right-looking algorithm is used, except for local contributions in the direct part where a left-looking scheme is applied. Some experiments have been performed and first results show that some substantial memory reductions can be achieved.
6. New Results

6.1. Low Mach number flows simulations issue
Participants: Pascal Bruel, Tarik Kousksou.

Since the targeted flows simulations (DNS) are by essence unsteady and at low Mach number, the use of a compressible solve has to be considered with great care. As a preliminary step towards the use of a fully implicit DG approach, we have joined the group of E. Dick at the Ghent University (Belgium) to help studying different aspects linked with low Mach number flow simulations [8], [7], [3]. The question of time consistency of the hyperbolic fluxes schemes for unsteady calculations has been dealt with and some pathological behavior of schemes such as the ones belonging to the AUSM family have been evidenced. A modification of AUSM+-up that satisfies the time-step dependency as well as the suitable scaling property of the pressure-velocity coupling evidenced has been proposed and tested [6].

6.2. Simulations of jets in crossflow
Participants: Pascal Bruel, Tarik Kousksou.

In order to prepare our benchmarking activity, we have been using the LES computer code AVBP (from Cerfacs and IFP) in order to simulate a multijet in crossflow configuration corresponding to the MAVERIC flow configuration. These simulations have been done in partnership with Turbomeca. The comparisons between LES and experiments is quite encouraging. An acoustic forcing technique has been used to establish a stationary acoustic wave inside the crossflow. The mass flow rate through the different holes proved to be significantly altered by the presence of the planar acoustic wave [4].

6.3. Discontinuous Galerkin methods for compressible multiphase flows
Participants: Vincent Perrier, Erwin Franquet.

We developed discontinuous Galerkin methods for compressible multiphase flows. This method is based on the method developed in [12] concerning the modelling of multiphase flows, and on the method developed in [36] concerning multiphase flows. In the method developed in [12], the exact expression of the continuous system is unclear, and as a consequence, the cell integral that naturally appear in the discontinuous Galerkin formulation is not clearly defined. In [2], [11], we developed an original analysis of the scheme [12] by mean of a stochastic process, which gave a unified framework for defining both the numerical scheme and the continuous limit. This was then applied to multiphase flows with phase transition in [10], [1]. Our method is currently being extended to interface flows with the maximum preserving limiter developed by [38].
5. New Results

5.1. New result 1

In [5], we explain the links between the solutions of the bidomain and monodomain models using some analytical arguments. The result is partially based on the theory of the bidomain operator explained in [2]. We can imagine several consequences to this general results, like improving the preconditionner proposed by C. Pierre [7] or derive some intermediate models.

5.2. New result 2

We computed some bidomain solutions for use by M. Pop and M. Sermesant in the STACOM’11 challenge from the MICCAI 2011 conference. They are the only bidomain simulations presented within this collaborative challenge. A collaborative paper will be published, see [8].
6. New Results

6.1. Models

6.1.1. Using the Last-mile Model as a Distributed Scheme for Available Bandwidth Prediction

Participants: Olivier Beaumont, Lionel Eyraud-Dubois, Young Won.

Several Network Coordinate Systems have been proposed to predict unknown network distances between a large number of Internet nodes by using only a small number of measurements. These systems focus on predicting latency, and they are not adapted to the prediction of available bandwidth. But end-to-end path available bandwidth is an important metric for the performance optimisation in many high throughput distributed applications, such as video streaming and file sharing networks. In [34], we propose to perform available bandwidth prediction with the last-mile model, in which each node is characterised by its incoming and outgoing capacities. This model has been used in several theoretical works for distributed applications. We design decentralised heuristics to compute the capacities of each node so as to minimise the prediction error. We show that our algorithms can achieve a competitive accuracy even with asymmetric and erroneous end-to-end measurement datasets. A comparison with existing models (Vivaldi, Sequoia, PathGuru, DMF) is provided. Simulation results also show that our heuristics can provide good quality predictions even when using a very small number of measurements.

6.1.2. Divisible Load Scheduling

Participants: Olivier Beaumont, Nicolas Bonichon, Lionel Eyraud-Dubois.

Malleable tasks are jobs that can be scheduled with preemptions on a varying number of resources. In [31], we focus on the special case of work-preserving malleable tasks, for which the area of the allocated resources does not depend on the allocation and is equal to the sequential processing time. Moreover, we assume that the number of resources allocated to each task at each time instant is bounded. We consider both the clairvoyant and non-clairvoyant cases, and we focus on minimizing the weighted sum of completion times. In the weighted non-clairvoyant case, we propose an approximation algorithm whose ratio (2) is the same as in the unweighted non-clairvoyant case. In the clairvoyant case, we provide a normal form for the schedule of such malleable tasks, and prove that any valid schedule can be turned into this normal form, based only on the completion times of the tasks. We show that in these normal form schedules, the number of preemptions per task is bounded by 3 on average. At last, we analyze the performance of greedy schedules, and prove that optimal schedules are greedy for a special case of homogeneous instances. We conjecture that there exists an optimal greedy schedule for all instances, which would greatly simplify the study of this problem. Finally, we explore the complexity of the problem restricted to homogeneous instances, which is still open despite its very simple expression. (Join work with Loris Marchal from ENS Lyon)

6.1.3. Modeling and Practical Evaluation of a Service Location Problem in Large Scale Networks

Participants: Olivier Beaumont, Nicolas Bonichon, Hubert Larchevêque.
In [33], we consider a generalization of a classical optimization problem related to server and replica location problems in networks. More precisely, we suppose that a set of users distributed over a network wish to have access to a particular service proposed by a set of providers. The aim is then to distinguish a set of service providers able to offer a sufficient amount of resources in order to satisfy the requests of the clients. Moreover, a quality of service following some requirements in terms of latencies is desirable. A smart repartition of the servers in the network may also ensure good fault tolerance properties. We model this problem as a variant of Bin Packing, namely Bin Packing under Distance Constraint (BPDC) where the goal is to build a minimal number of bins (i.e. to choose a minimal number of servers) so that (i) each client is associated to exactly one server, (ii) the capacity of the server is large enough to satisfy the requests of its clients and (iii) the distance between two clients associated to the same server is minimized. We prove that this problem is hard to approximate even when using resource augmentation techniques; we compare the number of obtained bins when using polynomial time algorithms allowed to build bins of diameter at most $\beta d_{\max}$, for $\beta > 1$, to the optimal number of bins of diameter at most $d_{\max}$. On the one hand, we prove that (i) if $\beta = (2 - \epsilon)$, BPDC is hard to approximate within any constant approximation ratio, for any $\epsilon > 0$; and that (ii) BPDC is hard to approximate at a ratio lower than $\frac{3}{2}$ even if resource augmentation is used. On the other hand, if $\beta = 2$, we propose a polynomial time approximation algorithm for BPDC with approximation ratio $\frac{7}{3}$ in the general case. We show how to turn an approximation algorithm for BPDC into an approximation algorithm for the non-uniform capacitated $K$-center problem and vice-versa. Then, we present a comparison of the quality of results for BPDC in the context of several Internet latency embedding tools such as Sequoia and Vivaldi, using datasets based on PlanetLab latency measurements.

6.1.4. Use of Internet Embedding Tools for Heterogeneous Resources Aggregation

Participants: Olivier Beaumont, Nicolas Bonichon, Philippe Duchon, Hubert Larchevêque.

In [28], we are interested in large scale distributed platforms like BOINC, consisting of heterogeneous resources and using the Internet as underlying communication network. In this context, we study a resource clustering problem, where the goal is to build clusters having at least a given capacity and such that any two participants to the same cluster are not too far from each other. In this context, the distance between two participants corresponds to the latency of a communication between them. Our goal is to provide algorithms with provable approximation ratios. In such large scale networks, it is not realistic to assume that the whole latency matrix (that gives the latency between any two participants) is known, and we need to rely on embedding tools such as Vivaldi or Sequoia. These tools enable to work on compact descriptions and well described metric spaces in which the distance between two points can be obtained directly from a small amount of information available at each node. We present the Bin Covering under Distance Constraint problem (BCDC for short), and propose dedicated algorithms for this problem for each metric space induced by each of the embedding tools. Then, we propose a comparison of these algorithms based on actual latency measures, that enables to decide which algorithm/embedding tool pair offers in practice for realistic datasets the best balancing between distance prediction and approximation ratios for the resource clustering problem.

6.1.5. Broadcasting on Large Scale Heterogeneous Platforms with Connectivity Artifacts under the Bounded Multi-Port Model

Participants: Olivier Beaumont, Nicolas Bonichon, Lionel Eyraud-Dubois, Przemyslaw Uznanski.

In [32], we consider the classical problem of broadcasting a large message at an optimal rate in a large scale distributed network. The main novelty of our approach is that we consider that the set of participating nodes can be split into two parts: "green" nodes that stay in the open-Internet and "red" nodes that lie behind firewalls or NATs. Two red nodes cannot communicate directly, but rather need to use a green node as a gateway for transmitting a message. In this context, we are interested in both maximizing the throughput (i.e. the rate at which nodes receive the message) and minimizing the degree at the participating nodes, i.e. the number of TCP connections they must handle simultaneously. We consider both cyclic and acyclic solutions for the flow graph. In the cyclic case, our main contributions are a closed form formula for the optimal cyclic throughput and the proof that the optimal solution may require arbitrarily large degrees. In the acyclic case, we propose an algorithm to achieve the optimal throughput with low degree. Then, we prove a worst case ratio between
the optimal acyclic and cyclic throughput and show through simulations that this ratio is on average very close to 1, which makes acyclic solutions efficient both in terms of throughput and of number of connections.

6.2. Overlays and distributed algorithms

6.2.1. Locally Fair Graph Exploration Strategies

Participants: David Ilcinkas, Ralf Klasing, Adrian Kosowski.

In [16], we considered the problem of exploring an anonymous undirected graph using an oblivious robot. The studied exploration strategies are designed so that the next edge in the robot’s walk is chosen using only local information, and so that some local equity (fairness) criterion is satisfied for the adjacent undirected edges. Such strategies can be seen as an attempt to derandomize random walks, and are natural counterparts for undirected graphs of the rotor-router model for symmetric directed graphs. The first of the studied strategies, known as Oldest-First (OF), always chooses the neighboring edge for which the most time has elapsed since its last traversal. Unlike in the case of symmetric directed graphs, we show that such a strategy in some cases leads to exponential cover time. We then consider another strategy called Least-Used-First (LUF) which always uses adjacent edges which have been traversed the smallest number of times. We show that any Least-Used-First exploration covers a graph $G = (V, E)$ of diameter $D$ within time $O(D|E|)$, and in the long run traverses all edges of $G$ with the same frequency.

6.2.2. Black Hole Search in Directed Graphs

Participant: Adrian Kosowski.

In [21] we considered a team of agents which has to explore a graph $G$ where some nodes can be harmful. Robots are initially located at the so called home base node. The dangerous nodes are the so called black hole nodes, and once a robot enters in one of them, it is destroyed. The goal is to find a strategy in order to explore $G$ in such a way that the minimum number of robots is wasted. The exploration ends if there is at least one surviving robot which knows all the edges leading to the black holes. As many variations of the problem have been considered so far, the solution and its measure heavily depend on the initial knowledge and the capabilities of the robots. We assume that $G$ is a directed graph, the robots are associated with unique identifiers, they know the number of nodes $n$ of $G$ (or at least an upper bound on $n$), and they know the number of edges $\Delta$ leading to the black holes. Each node is associated with a white board where robots can read and write information in a mutual exclusive way. A recently posed question (Czyzowicz et al. 2009) is whether some number of robots, expressed as a function of parameter Delta only, is sufficient to detect black holes in directed graphs of arbitrarily large order $n$. We give a positive answer to this question for the synchronous case, i.e., when the robots share a common clock, showing that $O(\Delta^2)$ robots are sufficient to solve the problem. This bound is nearly tight, since it is known that at least $2^\Delta$ robots are required for some instances. Quite surprisingly, we also show that unlike in the case of undirected graphs, for the directed version of the problem, synchronization can sometimes make a difference: for $\Delta = 2$, in the synchronous case 4 robots are always sufficient, whereas in the asynchronous case at least 5 robots are sometimes required.

6.2.3. Rendezvous for Location-Aware Agents

Participant: Adrian Kosowski.

In [35] we studied rendezvous of two anonymous agents, where each agent knows its own initial position in the environment. Their task is to meet each other as quickly as possible. The time of the rendezvous is measured by the number of synchronous rounds that agents need to use in the worst case in order to meet. In each round, an agent may make a simple move or it may stay motionless. We consider two types of environments, finite or infinite graphs and Euclidean spaces. A simple move traverses a single edge (in a graph) or at most a unit distance (in Euclidean space). The rendezvous consists in visiting by both agents the same point of the environment simultaneously (in the same round). In [35], we propose several asymptotically optimal rendezvous algorithms. In particular, we show that in the line and trees as well as in multi-dimensional Euclidean spaces and grids the agents can rendezvous in time $O(d)$, where $d$ is the distance between the initial
positions of the agents. The problem of location-aware rendezvous was studied before in the asynchronous model for Euclidean spaces and multi-dimensional grids, where the emphasis was on the length of the adopted rendezvous trajectory. We point out that, contrary to the asynchronous case, where the cost of rendezvous is dominated by the size of potentially large neighborhoods, the agents are able to meet in all graphs of at most $n$ nodes in time almost linear in $d$, namely, $O(d \log^2 n)$. We also determine an infinite family of graphs in which synchronized rendezvous takes time $\Omega(d)$.

6.2.4. Boundary Patrolling by Mobile Agents

**Participant:** Adrian Kosowski.

In the boundary patrolling problem, a set of $k$ mobile agents are placed on the boundary of a simply connected planar object represented by a cycle of unit length. Each agent has its own predefined maximal speed, and is capable of moving around this boundary without exceeding its maximal speed. The agents are required to protect the boundary from an intruder which attempts to penetrate to the interior of the object through a point of the boundary, unknown to the agents. The intruder needs some time interval of length $\tau$ to accomplish the intrusion. Will the intruder be able to penetrate into the object, or is there an algorithm allowing the agents to move perpetually along the boundary, so that no point of the boundary remains unprotected for a time period $\tau$? Such a problem may be solved by designing an algorithm which defines the motion of agents so as to minimize the idle time $I$, i.e., the longest time interval during which any fixed boundary point remains unvisited by some agent, with the obvious goal of achieving $I < \tau$. Depending on the type of the environment, this problem is known as either boundary patrolling or fence patrolling in the robotics literature. The most common heuristics adopted in the past include the cyclic strategy, where agents move in one direction around the cycle covering the environment, and the partition strategy, in which the environment is partitioned into sections patrolled separately by individual agents. We have obtained, to our knowledge, the first study of the fundamental problem of boundary patrolling by agents with distinct maximal speeds. In this scenario, we give special attention to the performance of the cyclic strategy and the partition strategy. In [36], we propose general bounds and methods for analyzing these strategies, obtaining exact results for cases with 2, 3, and 4 agents. We show that there are cases when the cyclic strategy is optimal, cases when the partition strategy is optimal and, perhaps more surprisingly, novel, alternative methods have to be used to achieve optimality.

6.2.5. Rendezvous in trees

**Participant:** Adrian Kosowski.

In the rendezvous problem in trees, two identical (anonymous) mobile agents start from arbitrary nodes of an unknown tree and have to meet at some node. Agents move in synchronous rounds: in each round an agent can either stay at the current node or move to one of its neighbors. We consider deterministic algorithms for this rendezvous task. In [51] we have presented a tight trade-off between the optimal time of completing rendezvous and the size of memory of the agents. For agents with $k$ memory bits, we show that optimal rendezvous time is $\Theta(n + n^2/k)$ in $n$-node trees. More precisely, if $k \geq c \log n$, for some constant $c$, we design agents accomplishing rendezvous in arbitrary trees of unknown size $n$ in time $O(n + n^2/k)$, starting with arbitrary delay. We also show that no pair of agents can accomplish rendezvous in time $o(n + n^2/k)$, even in the class of lines of known length and even with simultaneous start. Finally, we prove that at least logarithmic memory is necessary for rendezvous, even for agents starting simultaneously in a $n$-node line.

6.2.6. How many oblivious robots can explore a line

**Participant:** David Ilcinkas.

In [20] we consider the problem of exploring an anonymous line by a team of $k$ identical, oblivious, asynchronous deterministic mobile robots that can view the environment but cannot communicate. We completely characterize sizes of teams of robots capable of exploring a $n$-node line. For $k < n$, exploration by $k$ robots turns out to be possible, if and only if either $k = 3$, or $k \geq 5$, or $k = 4$ and $n$ is odd. For all values of $k$ for which exploration is possible, we give an exploration algorithm. For all others, we prove an impossibility result.
6.2.7. Asynchronous deterministic rendezvous in bounded terrains

Participant: David Ilcinkas.

Two mobile agents (robots) have to meet in an a priori unknown bounded terrain modeled as a polygon, possibly with polygonal obstacles. Robots are modeled as points, and each of them is equipped with a compass. Compasses of robots may be incoherent. Robots construct their routes, but the actual walk of each robot is decided by the adversary that may, e.g., speed up or slow down the robot. In [18], we consider several scenarios, depending on three factors: (1) obstacles in the terrain are present, or not, (2) compasses of both robots agree, or not, (3) robots have or do not have a map of the terrain with their positions marked. The cost of a rendezvous algorithm is the worst-case sum of lengths of the robots’ trajectories until they meet. For each scenario we design a deterministic rendezvous algorithm and analyze its cost. We also prove lower bounds on the cost of any deterministic rendezvous algorithm in each case. For all scenarios these bounds are tight.

6.2.8. On the Power of Waiting when Exploring Public Transportation Systems

Participants: David Ilcinkas, Ahmed Mouhamadou Wade.

We study the problem of exploration by a mobile entity (agent) of a class of dynamic networks, namely the periodically-varying graphs (the PV-graphs, modeling public transportation systems, among others). These are defined by a set of carriers following infinitely their prescribed route along the stations of the network. Flocchini, Mans, and Santoro [58] (ISAAC 2009) studied this problem in the case when the agent must always travel on the carriers and thus cannot wait on a station. They described the necessary and sufficient conditions for the problem to be solvable and proved that the optimal number of steps (and thus of moves) to explore a \( n \)-node PV-graph of \( k \) carriers and maximal period \( p \) is in \( \Theta(k \cdot p^2) \) in the general case.

In [46], we study the impact of the ability to wait at the stations. We exhibit the necessary and sufficient conditions for the problem to be solvable in this context, and we prove that waiting at the stations allows the agent to reduce the worst-case optimal number of moves by a multiplicative factor of at least \( \Theta(p) \), while the time complexity is reduced to \( \Theta(n \cdot p) \). (In any connected PV-graph, we have \( n \leq k \cdot p \).) We also show some complementary optimal results in specific cases (same period for all carriers, highly connected PV-graphs). Finally this new ability allows the agent to completely map the PV-graph, in addition to just explore it.

6.2.9. The impact of edge deletions on the number of errors in networks

Participants: Christian Glacet, Nicolas Hanusse, David Ilcinkas.

In [41], we deal with an error model in distributed networks. For a target \( t \), every node is assumed to give an advice, i.e. to point to a neighbor that take closer to the destination. Any node giving a bad advice is called a liar. Starting from a situation without any liar, we study the impact of topology changes on the number of liars.

More precisely, we establish a relationship between the number of liars and the number of distance changes after one edge deletion. Whenever \( \ell \) deleted edges are chosen uniformly at random, for any graph with \( n \) nodes, \( m \) edges and diameter \( D \), we prove that the expected number of liars and distance changes is \( O(\ell^2Dn/m) \) in the resulting graph. The result is tight for \( \ell = 1 \). For some specific topologies, we give more precise bounds.

6.2.10. Computations in interconnection networks with a shared whiteboard

Participant: Adrian Kosowski.

In [52], We study the computational power of graph-based models of distributed computing in which each node additionally has access to a global whiteboard. A node can read the contents of the whiteboard and, when activated, can write one message of \( O(\log n) \) bits on it. A message is only based on the local knowledge of the node and the current content of the whiteboard. When the protocol terminates, each node computes the output based on the final contents of the whiteboard in order to answer some question on the network’s topology. We propose a framework to formally define several scenarios modelling how nodes access the whiteboard, in a synchronous way or not. This extends the work of Becker et al. where nodes were imposed to create their messages only based on their local knowledge (i.e., with the whiteboard empty). We prove that the four
models studied have increasing power of computation: any problem that can be solved in the weakest one can be solved in the second, and so on. Moreover, we exhibit problems that separate models, i.e., that can be solved in one model but not in a weaker one. These problems are related to Maximal Independent Set and detection of cycles. Finally we investigate problems related to connectivity as the construction of spanning- or BFS-tree in our different models.

6.2.11. Network Verification

Participant: Ralf Klasing.

In [27], we address the problem of verifying the accuracy of a map of a network by making as few measurements as possible on the nodes of the network. In the past, this task has been formalized as an optimization problem that, given a graph \( G = (V, E) \), asks for finding a minimum-size subset \( Q \) of vertices of \( G \) such that the information returned by the queries on \( Q \) uniquely identifies \( G \). Previously, two global query models have been studied. In [27], we propose a query model that uses only local knowledge about the network. Quite naturally, we assume that a query at a given node \( q \) returns the associated routing table, namely a set of entries which provides, for each destination node, a corresponding (set of) first-hop node(s) along an underlying shortest path. First, we show that any network of \( n \) nodes needs \( \Omega(\log \log n) \) queries to be verified. Then, we prove that there is no \( o(\log n) \) approximation algorithm for the problem, unless \( P = \text{NP} \), even for graphs with diameter 2. On the positive side, we provide an \( O(\log n) \)-approximation algorithm to verify a network of diameter 2, and we give exact polynomial-time algorithms for paths, trees and cycles of even length.

6.3. Compact and distributed data structures

6.3.1. Query optimization in databases

Participants: Nicolas Hanusse, Sofian Maabout.

Datacubes are data structures designed to query optimization in databases. In [42] we provide some algorithmic solutions in a user centric setting: the request time is guaranteed and the amount of memory space is minimized.

6.3.2. Parallel computations of Borders

Participants: Nicolas Hanusse, Sofian Maabout.

Borders are fundamental building blocks in data mining. They are used to find frequent patterns, dependencies between attributes, ... In [43] we provide an algorithm that computes borders with a speedup of \( p \) (under reasonable hypothesis) for \( p \) cores.

6.3.3. Node-disjoint multipath spanners and their relationship with fault-tolerant spanners

Participants: Cyril Gavoille, Quentin Godfroy.

Motivated by multipath routing, we introduce a multi-connected variant of spanners. For that purpose we introduce in [40] the \( p \)-multipath cost between two nodes \( u \) and \( v \) as the minimum weight of a collection of \( p \) internally vertex-disjoint paths between \( u \) and \( v \). Given a weighted graph \( G \), a subgraph \( H \) is a \( p \)-multipath \( s \)-spanner if for all \( u, v \), the \( p \)-multipath cost between \( u \) and \( v \) in \( H \) is at most \( s \) times the \( p \)-multipath cost in \( G \). The \( s \) factor is called the stretch.

Building upon recent results on fault-tolerant spanners, we show how to build \( p \)-multipath spanners of constant stretch and of \( O(n^{1+1/k}) \) edges, for fixed parameters \( p \) and \( k \), \( n \) being the number of nodes of the graph. Such spanners can be constructed by a distributed algorithm running in \( O(k) \) rounds.

Additionally, we give an improved construction for the case \( p = k = 2 \). Our spanner \( H \) has \( O(n^{3/2}) \) edges and the \( p \)-multipath cost in \( H \) between any two node is at most twice the corresponding one in \( G \) plus \( O(W) \), \( W \) being the maximum edge weight.
6.3.4. On approximate distance labels and routing schemes with affine stretch

**Participant:** Cyril Gavoille.

For every integral parameter $k > 1$, given an unweighted graph $G$, we construct in polynomial time in [25], for each vertex $u$, a distance label $L(u)$ of size $O(n^{2/(2k-1)})$. For any $u, v \in G$, given $L(u), L(v)$ we can return in time $O(k)$ an affine approximation $\hat{d}(u, v)$ on the distance $d(u, v)$ between $u$ and $v$ in $G$ such that $d(u, v) - \hat{d}(u, v) \leq (2k-2)d(u, v) + 1$. Hence we say that our distance label scheme has affine stretch of $(2k-2)d + 1$. For $k = 2$ our construction is comparable to the $O(n^{5/3})$ size, $2d + 1$ affine stretch of the distance oracle of Pătraşcu and Roditty (FOCS '10), it incurs a $o(\log n)$ storage overhead while providing the benefits of a distance label.

For any $k > 1$, given a restriction of $o(n^{1/(k-1)})$ on the total size of the data structure, our construction provides distance labels with affine stretch of $(2k-2)d + 1$ which is better than the stretch $(2k-1)d$ scheme of Thorup and Zwick (J. ACM '05).

Our second contribution is a compact routing scheme with poly-logarithmic addresses that provides affine stretch guarantees. With $O(n^{3/(3k-2)})$-bit routing tables we obtain affine stretch of $(4k-6)d + 1$, for any $k > 1$.

Given a restriction of $o(n^{1/(k-1)})$ on the table size, our routing scheme provides affine stretch which is better than the stretch $(4k-5)d$ routing scheme of Thorup and Zwick (SPAA '01).

6.3.5. Sparse spanners vs. compact routing

**Participant:** Cyril Gavoille.

Routing with multiplicative stretch 3 (which means that the path used by the routing scheme can be up to three times longer than a shortest path) can be done with routing tables of $O(n)$ return in time.

Routing with multiplicative stretch 3 (which means that the path used by the routing scheme can be up to three times longer than a shortest path) can be done with routing tables of $O(n)$ return in time.

Routing with tables of size $O(n)$ for general graphs, and the above bound of $n^{1/3}$ on the stretch and the routing table size holds for all graphs of linear local tree-width, a class of graphs including bounded-genus graphs and apex-minor-free graphs.

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3Tilde-big-$\mathcal{O}$ notation is similar to big-$\mathcal{O}$ notation up to factors poly-logarithmic in $n$.
6. New Results

6.1. Convergence of adaptive finite element algorithms

Participants: Roland Becker, Shipeng Mao, David Trujillo.

The theoretical analysis of mesh-adaptive methods is a very active field of research. We have generalized our previous results concerning optimality of adaptive methods to nonconforming finite elements [49]. Our results include the error due to iterative solution of the system matrices by means of a simple stopping criterion related to the error estimator. The main difficulty was the treatment of the nonconformity which leads to a perturbation of the orthogonality relation at the heart of the proofs for conforming finite elements. We have been able to extend this result to the Stokes equations, considering different lowest-order nonconforming finite elements on triangular and quadrilateral meshes [16].

In [17] we have shown that the smallness assumption required in all former proofs of optimality of adaptive finite element methods can be overcome, at least in some situations.

Finally, we have shown optimality of a new goal-oriented method in [19].

Our theoretical studies, which are motivated by the aim to develop better adaptive algorithms, have been accompanied by software implementation with the Concha library, see Section 5.1. It hopefully opens the door to further theoretical and experimental studies.

6.2. Finite element methods for interface problems

Participants: Nelly Barrau, Roland Becker, Robert Luce, Erik Burman, Peter Hansbo.

The original formulation of NXFEM [62] is based on the doubling of elements. In some situations, as the case of a moving interface, it is computationally more convenient to have a method with local enrichment, as for the standard XFEM. In [41] we have developed such an approach based on NXFEM. We have developed an hierarchical formulation for a fictitious domain formulation in [13].

One of the technical difficulties is the simultaneous robustness of the method with respect to the size of the intersection of a mesh cell with the interface and with respect to the discontinuous diffusion parameters. This is the subject of the thesis of Nelly Barrau, supervised by Robert Luce and Eric Dubach (LMAP).

6.3. Discontinuous finite element methods

Participants: Roland Becker, Daniela Capatina, Julie Joie.

We have developed a new discontinuous Galerkin scheme for the Stokes equations and corresponding three-fields formulation. In this work, which is part of the Phd Thesis of Julie Joie, we introduce a modification of the stabilization term in the standard DG-IP method. This allows for a cheaper implementation and has a more robust behavior with respect to the stabilization parameter; we have shown convergence towards the solution of non-conforming finite element methods for linear, quadratic and cubic polynomial degrees. This scheme has been extended to the three-field formulation of the Stokes problem, which is a further step towards the polymer project of Section 4.2. Since it is well known that the non-conforming finite element approximations do not verify the discrete Korn inequality, an appropriate further stabilization term is introduced, see [42].

6.4. Stabilized finite element methods

Participants: Roland Becker, Erik Burman, Peter Hansbo.
We have developed a new stabilized finite element formulation based on implicit penalization of the singularities of higher-order derivatives of continuous finite element spaces in [12]. It has been applied to the convection-diffusion problem as well as to the incompressible Euler equations.

6.5. **A posteriori error estimators based on $H(\text{div})$-reconstructed fluxes**

**Participants:** Roland Becker, Daniela Capatina, Robert Luce.

Mesh adaptivity is nowadays an essential tool in numerical simulations; in order to achieve it, reliable and efficient, easily computable *a posteriori* error estimators are needed. Such estimators obtained by reconstructing locally conservative fluxes in the Raviart-Thomas finite element space have been largely employed in the past years.

We have so far considered the convection-diffusion equation and proposed a unified framework for several finite element approximations (conforming, nonconforming and discontinuous Galerkin). The main advantage of our approach is to use, contrarily to the existing references, only the primal mesh for the flux reconstruction, which presents certain facilities from a computational point of view.

For this purpose, the construction of the $H(\text{div})$-vector involved in the error estimator is inspired by the hypercircle method cf. [53] and is achieved on patches, which may overlap. A patch depends on the type of the employed finite elements and is defined as the support of a basis function.

Our first results were presented in [26]. We are working on the extension to higher-order approximations, to quadrilateral meshes and to other model problems.

6.6. **A posteriori error analysis of sensitivities**

**Participants:** Roland Becker, Daniela Capatina, Robert Luce, David Trujillo.

Most practical applications involve parameters $q = (q_i)_{1 \leq i \leq N}$ of different origins: physical (viscosity, heat conduction), modeling (computational domain, boundary conditions) and numerical (mesh, stabilization parameters, stopping criteria, values of a turbulence model). Numerical simulations can provide information related to the (first order) sensitivity of a quantity of physical interest $I(q)$ with respect to different parameters: $\partial I/\partial q_i$. Their computation can help to validate the physical model, to explain unexpected behaviour and also to guide efforts to improve both the physical and the computational models.

*A posteriori* error estimates for the functional itself, for fixed values of the parameters $q$, are well-known, cf. for example [47] where a goal-oriented error control is achieved by introducing an adjoint problem. Our goal is to provide a general framework for the *a posteriori* error estimation of sensitivities $\partial I/\partial q_i - \partial I_h/\partial q_i$, which has not been given yet in the literature.

So far, we have applied the proposed method to the computation of the Nusselt number measuring the efficiency of a cooling process, described in the project Optimal. A cold liquid is injected in a annular domain in order to cool a heated interior stator.

First numerical results, including adaptation with respect to the functional and to the sensitivity, have been carried out with the library Concha. They have been presented in [33], [30]. In Figure 10 one may see the computed temperature and velocity field, while the *a posteriori* error estimator for the sensitivity of the Nusselt number with respect to the inflow speed at the right-hand side inlet, as well as the adapted mesh, are given in Figure 11.

In the future, several important aspects related to the adaptive method are still to be investigated such as design of an appropriate adaptive algorithm, proof of its convergence and optimality etc.

6.7. **Viscoelastic fluids modeling and numerical simulation**

**Participants:** Roland Becker, Daniela Capatina, Didier Graebling, Julie Joie.

We have continued our activities with respect to numerical simulations of polymer flows.
Figure 10. Computed velocity and temperature fields.

Figure 11. Error estimator for the sensitivity and adapted mesh.
We have further validated [32] the code on both triangular and quadrilateral 2D meshes, by using a mixed non-conforming/DG method. In the case of Giesekus model, comparisons of velocity profile with semi-analytical solutions for Poiseuille flow [70] and with experimental data [73] for the 4:1 contraction are respectively shown in Figures 12 and 13.

The quadrilateral scheme needs an additional stabilization term, in order to ensure uniform consistency and stability for the underlying linear problem. It has been tested in particular on the benchmark case of flow around a 2D cylinder, for which our code converged for high values of the Weissenberg number (We > 70).

We have computed the drag and compared it, see Figure 14, with numerical data found in the literature [58], [65], [76], [57] in the case of the Oldroyd-B model.

The system associated to this quasi-linear model has been solved on rather fine meshes (of about $10^6$ elements) thanks to a multigrid solver based on a Vanka type preconditioner. We have worked on the extension of the multigrid method to more complex and more realistic polymer models, involving nonlinear terms in the constitutive law such that Phan Thien-Tanner and Giesekus models.

The unsteady case has also been treated for different geometries.

The parallelization of the library is ongoing work as described in the section 5.3; first tests have been carried on in the case of viscoelastic liquids.

In order to better describe real polymer flows, the thermal aspects have to be taken into account. As a first step, the coupling of the flow with the energy equation in the Newtonian case was considered in [38], by using a conservative variable. Our next objective is to simulate anisothermal viscoelastic flows, including typical effects such that thermo-dependent viscosity and viscous heating.

With these tools, the long-term goal is to successively build up robust and efficient software in order to tackle design problems.

Moreover, we intend to consider other models of non-Newtonian fluids employed in other application domains such as biomedicine.

6.8. Positivity preserving schemes

Participants: Roland Becker, Daniela Capatina.
Figure 13. Comparison with experimental data for the 4:1 contraction.

Figure 14. Comparison of drag coefficients with the literature.
The stability and robustness with respect to physical parameters of numerical schemes for polymer flows is a challenging question. Indeed, most algorithms encounter serious convergence problems for large Weissenberg numbers. In the recent years, this issue has been associated to the discrete positive definiteness of the so-called conformation tensor. It seems therefore essential for the numerical simulations to employ positivity preserving schemes.

In order to develop such schemes, we have adopted the approach proposed by Lee and Xu [68] in the case of the quasi-linear Oldroyd-B model, based on the similarities between its constitutive equation and differential Riccati equations. We have applied it to a more general matrix equation; a typical example is the nonlinear Giesekus constitutive law. In agreement with our code (see Section 6.7), we have discretized it by a discontinuous Galerkin method combined with an upwinding of the transport terms, whereas the approach of Lee and Xu relies essentially on the characteristics method.

We have shown that a modification of Newton’s method yields a monotone and positive scheme, under certain hypothesis, and we have applied this study to both Oldroyd-B and Giesekus polymer models. This allowed us to better understand and explain the better behaviour of the latter for large Weissenberg numbers. These results have been presented in [24],[31].

We are working on several challenging questions such as the extension to other discretization methods, the improvement of the iterative method or the derivation of energy estimates for the coupled system.

6.9. Discretization of Euler’s equations

Participants: Roland Becker, Kossivi Gopki, Eric Schall, David Trujillo.

Over the past years, significant advances have been made in developing discontinuous Galerkin finite element methods (DGFEM) for applications in fluid flow and heat transfer. Certain features of the method have made it attractive as an alternative to other popular methods such as finite volume and more convenient finite element methods in thermal fluid engineering analyses. The DGFEM has been used successfully to solve hyperbolic systems of conservation laws. It makes use of the same local function space as the continuous method, but with relaxed continuity at inter-element boundaries. Since it uses discontinuous piecewise polynomial bases, the discretization is locally conservative and in the considered lowest-order case, the method preserves the maximum principle for scalar equations.

One of the challenges in Computational Fluid Dynamic (CFD) is to obtain as accurate as possible the solution of the problem under consideration at very low cost in terms of computational time. So our principal work is to find some relevant and robust strategies and technics of meshes adaptation in order to concentrate just the calculation where there are physical phenomena to capture. From Industrial point of view, the aim is to get the stationary solution as quick as possible with as much accuracy as possible. The main limitation of these results in CFD concern the underlying models: for example, nearly nothing seems to be known for (even linear) first-order systems or for realistic nonlinear equations. We therefore have developed different modern techniques, especially adaptive methods, to tackle this kind of problems in compressible CFD. The strategy is to iteratively improve the quality of the approximate solutions based on computed information (a posteriori error analysis). In this way, a sequence of locally refined meshes is constructed, which allows for better efficiency as compared to more classical approaches in the presence of different kind of singularities. The main goal is to improve the aerodynamical design process for complex configurations by significantly reducing the time from geometry to solution at engineering-required accuracy using high-order adaptive methods.

One of our strategies of refinement is based on the creation of hanging nodes commonly called non-conforming refinement. The figures 15 show superposition of two kinds of meshes. One is a non-conforming refined mesh (black color) and the other one is the initial grid (red color) on which the refinement has been performed. It shows the technic of cutting the cells where singularities occur in the scramjet inlet.

The mesh adaptation is designed using some criteria as a posteriori error estimates. We have designed criteria based on the calculation of the jump of physical quantities like density, pressure, entropy, temperature and mach number at the inter-element. This criteria seems to be a very good indicator for the mesh adaptation. Figure 16 is the comparison of isoline of the density in scramjet internal flow at mach 3 of the initial mesh,
Figure 15. Superposition of non-conforming adapted black color) grid and initial grid (red color) – (a) quadrangles and (b) triangles.

The third and the sixth mesh after refinement. The indicator used is the density jump. It shows the impact and the accuracy of the solution obtained after the sixth iteration of the refinement.

Figure 16. Cutlines along the symmetry axis of various meshes for the scramjet test case

The figure shows the streamlines of the density in the scramjet inlet after the seventh iteration. This shows how the adaptation depicts almost clearly and accurately the shock waves and the expansion waves and their interactions in the domain.
Figure 17. Density streamlines on grid obtained after the seventh iteration of adaptive refinement procedure with density jump as indicator.

Figure 18 represent the density isolines of a flow past cylinder test case using the non-conforming mesh adaptation with quadrangular and triangular grids.

(a)  (b)

Figure 18. Locally adapted mesh on quadrilaterals (a) and triangles (b).

We have also settled another indication which is hierarchical. It measures the difference of $\frac{g_h}{2}$ with the physical quantity $\frac{g_{h/2}}{2}$ obtained by computation on a globally refined mesh $\frac{h}{2}$. This allows us to make a comparison.
with the previous indicator. The case test considered for this comparison is an external flows past a cylinder airfoil at fixed free stream conditions: $M_\infty = 3$. The result is quite surprising the way one type of indicator can capture phenomenon that are not capture by the another one. In fact the hierarchical indicator seems to capture recirculation downstream to the obstacle which was not capture by the jump indicator (see figure 19).

![Figure 19. Streamlines coloured by the density on meshes generated with hierarchical indicator (a) and with jump indicator (b)]

We compare the computational time between a non-conforming mesh refinement and a globally mesh refined with nearly the same amount of cells. The meshes contain quadrangles or triangles. We can observe through the following tables that the adapted meshes wether triangular or quadrangular meshes allow to save 20 to 90 times the computational time than the normal globally refined mesh. (see tables 1 and 2)

<table>
<thead>
<tr>
<th>Scramjet test case at mach=3</th>
<th>Flow past cylinder test case at mach=3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Table 1</strong></td>
<td><strong>Table 2</strong></td>
</tr>
<tr>
<td>Nodes</td>
<td>Cells</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>Scram_Quad_4</td>
<td>17003</td>
</tr>
<tr>
<td>Scram_Quad_Uniform</td>
<td>17183</td>
</tr>
<tr>
<td>Scram_Tri_4</td>
<td>9951</td>
</tr>
<tr>
<td>Scram_Tri_Uniform</td>
<td>13295</td>
</tr>
</tbody>
</table>

In table 1, the gain in time is 35 times in quadrangular grid case and 90 times triangular ones and in table 2, the gain in time: 18 times in quadrangular grid case and 58 times triangular ones. So one can say that the adaptive mesh with the strategies and technics we have settled are efficient and robust in capturing physical phenomenon at a very reasonable low cost.

In concluding, the procedure of refinement permit to save computational time and have good accuracy of the approximated solution computed. Our focus is to continue the improve our methods and strategies in order to meet the requirement of accuracy, robustness and efficiency. Many other works are in hand such as slope limiters for high-order Discontinous Galerkin, low mach number computation with some remarkable approaches.
6. New Results

6.1. On the Existence of Strict Optimal Controls for Constrained, Controlled Markov Processes in Continuous-Time

Participant: François Dufour.

Closedness and convexity conditions are identified under which optimal controls in the class of strict controls exist for a large class of stochastic processes under infinite-horizon discounted, long-term average, first exit, finite-horizon and discretionary stopping criteria in the presence of hard and/or soft constraints. The results are more general than results obtained by Haussmann and Lepeltier for a controlled diffusion under a mixed optimal-stopping/finite-horizon/first-exit criterion. The approach taken in this work is to utilize equivalent linear programming formulations of the control problems which provides a unified LP formulation for the problems. The conditions of Haussmann and Lepeltier are shown to imply the sufficient conditions of this paper when the process is a controlled diffusion. Simpler conditions are also identified for Markov chains, simple Markov jump processes, diffusions with jumps, regime-switching diffusions and solutions to Levy stochastic differential equations.

These results have been obtained in collaboration with Richard Stockbridge, Department of Mathematical Sciences, University of Wisconsin Milwaukee, USA. It has been accepted for publication in Stochastics [14].

6.2. Approximation of Markov Decision Processes with General State Space

Participant: François Dufour.

In this work, we deal with a discrete-time finite horizon Markov decision process with locally compact Borel state and action spaces, and possibly unbounded cost function. Based on Lipschitz continuity of the elements of the control model, we propose a state and action discretization procedure for approximating the optimal value function and an optimal policy of the original control model. We provide explicit bounds on the approximation errors. Our results are illustrated by a numerical application to a fisheries management problem.

These results have been obtained in collaboration with Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED, Madrid, Spain. It has been accepted for publication in Stochastics [13].

6.3. Asymmetry tests for Bifurcating Auto-Regressive Processes with missing data

Participants: Benoîte de Saporta, Anne Gégout-Petit.

Using the properties of the estimators studied in [20], we have constructed symmetry tests for bifurcating autoregressive processes (BAR) when some data are missing. BAR processes typically model cell division data. Each cell can be of one of two types odd or even. The goal of this work is to test asymmetry between odd and even cells in a single observed lineage. We have also derived asymmetry tests for the lineage itself, modeled by a two-type Galton-Watson process observed in a non standard scheme. We present applications on both simulated and real data.

This work is in collaboration with Laurence Marsalle of Lille 1 university. It will be soon submitted for publication.

6.4. Statistical study of asymmetry in cell lineage data

Participants: Benoîte de Saporta, Anne Gégout-Petit.
Simulation studies of the asymmetry in a single lineage data have shown a lack of power of the tests when the number of available generation is limited. This work proposes a rigorous methodology to study cell division data in the context of observation of several lineages. It generalizes [20]. We model the data by an asymmetric bifurcating autoregressive (BAR) process and take into account possibly missing data by modeling the genealogies with a two-type Galton Watson (GW) process. Our inference is based on several lineages, i.e. independent and identically distributed replicas of the coupled BAR and GW processes. We propose a least-squares estimator of the unknown parameters of the BAR process and an estimator of the parameters of the GW process, study their asymptotic properties and propose symmetry tests. Our results are applied on real data of Escherichia coli division.

This work is in collaboration with Laurence Marsalle of Lille 1 university. It will be soon submitted for publication.

6.5. Estimation of the jump rate of a PDMP

Participants: Romain Azaïs, François Dufour, Anne Gégout-Petit.

We estimate the jump rate of PDMP. We suppose the flow given by physics laws and we want to make some inference on \( \lambda \). \( \phi \) being deterministic, the problem can be rewritten as a problem of estimation of the rate \( \lambda(z, t) \) with \( z \in E \) with \( E \) an open set of a separable metric space. We have an ergodicity assumption on the observed PDMP and the asymptotic is in the time of observation of the process.

We distinguish three cases:

1. \( E \) is finite. In this case, we easily estimate each of the cumulated risk functions \( \Lambda(z, t) = \exp(- \int_0^t \lambda(z, s)ds) \) corresponding to each of \( z \in E \) by a Nelson Aalen estimator. The results is based on the decomposition in semi-martingale of the following counting process in an appropriate filtration:

\[
\forall t \geq 0, \quad N_n(z, t) = \sum_{i=0}^{n-1} \mathbf{1}_{\{S_{i+1} \leq t\}} \mathbf{1}_{\{Z_i = z\}},
\]

We obtain the estimator of the rate \( \lambda(z, t) \) by smoothing of the estimator of \( \Lambda \).

2. \( E \) is an open set of a general separable metric space but the transition measure \( Q \) does not depend on the time spent in the current regime. In this case, we suppose the rate \( \lambda(z, t) \) Lipschitz and the process ergodic with a stationary law denoted by \( \nu \). We first construct an estimation of the cumulated rate knowing that \( z \) belongs to a set \( A \) such that \( \nu(A) > 0 \) by:

\[
\hat{L}_n(A, t) = \sum_{i=0}^{n-1} \frac{1}{Y_n(A, S_{i+1})} \mathbf{1}_{\{S_{i+1} \leq t\}} \mathbf{1}_{\{Z_i \in A\}}
\]

We show the consistence of the estimator. Smoothing \( \hat{L}_n(A, t) \) and using a fine partition of \( E \) allow us to obtain an uniform result for the approximation of the rate \( \lambda(z, t) \), in some sense in \( t \) and \( z \).

3. \( E \) is an open set of a general separable metric space and the transition measure \( Q \) depends on the time spent in the current regime. Here, we loose some conditional independence between the \( S_i \)'s and the whole set of the locations of the jump \( \{Z_1, ..., Z_n\} \). We have to make a detour for the estimation of the law of the time \( S_{k+1} \) knowing the current \( Z_k \) by the the law \( S_{k+1} \) knowing \( (Z_k, Z_{k+1}) \). The method gives an estimation of the conditional density of \( S_{k+1} \) given \( Z_k \).

We have made simulation studies that give expected results. A R package for this estimation method is in progress.
6.6. Detection of a damaged operating mode of optronic equipment using Hidden Markov Model

Participants: Camille Baysse, Anne Gégout-Petit, Jérôme Saracco.

As part of optimisation of the reliability, Thales Optronics now includes systems that examine the state of its equipment. This function is performed by HUMS (Health & Usage Monitoring System). The aim is to implement a program based on these observations that can determine the lifetime of this optronic equipment and optimize its maintenance.

Our study focuses on a simple example of HUMS. As part of our research, we are interested in a variable called "time-to cold" noted TMF, which reflects the state of the system. Using these informations about this variable, we seek to detect as soon as possible a damaged state and propose a maintenance before failure. This would allow the Thales Optronics company to improve its maintenance system and achieve many economies.

For this we use a hidden Markov model. The state of our system at time t is then modeled by a continuous time Markov chain X(t) with three states: stable, damaged and failure. However we do not observe directly this chain but indirectly through the TMF, a noisy function of this chain. Thanks to filtering equations, we obtained results on the probability that an equipment is in a damaged state at time t, knowing the history of the TMF until this moment. We have subsequently studied the method on simulated data, before applying these results on the analysis of our real data and we have checked that the results are consistent with the reality. This work will be used by Thales Optronique for the optimization of the maintenance.

This work is a part of the CIFRE PhD Thesis of Camille Baysse founded by Thales Optronique. It is the object of a technical report [48] and was presented in [29] in an internal Thales seminar.

6.7. Optimal quantization applied to Sliced Inverse Regression

Participants: Romain Azaïs, François Dufour, Anne Gégout-Petit, Jérôme Saracco.

We tackle the well known Slice Inverse Regression (SIR) method for a semiparametric regression model involving a quantitative variable X and including a dimension reduction of X via a parameter β. The response variable Y is real. Our goal is to estimate β and to predict the response variable conditionally to X. We adapt SIR method using optimal quantization [57] in the first time only for the independent variable X for the estimation of β. In a second time, we quantize the variable (β̂n, Y) in order to propose a discrete conditional law of Y given X = x. We show the convergence of the estimator of β and of the conditional law. Simulation studies show the numerical qualities of our estimates. This work is the object of a publication in Journal of Statistical Planning and Inference [15] and was presented in a national conference [23].

6.8. Multivariate Analysis for the detection of the effect of a treatment

Participant: Anne Gégout-Petit.

The aim of this work is to give some statistical rules to determine if a patient is meeting a given treatment (a BD here). The criterium commonly used to determine if a patient is meeting a BD treatment is based only on one physiological parameter: if this parameter increases, the patient is meeting. But now, many physiological parameters are measured in routine and physiologists "ont le sentiment" that a patient could have a global amelioration of his health state due to the treatment without an increase of the single used parameter.
Using the measures of six variables before and after the treatment, the expected value of this variable under the hypothesis of good health, we first propose indices of amelioration. Using standard multivariate analysis techniques, we first study the correlation between these indices. We use classification in order to constitute groups of patients whose present homogeneous treatment responses. The method used on a cohort of 100 subjects gives three groups: in the first one, the mean of the indices is near zero, the treatment has no effect. In the second one, subjects present significant amelioration regarding two of the indices but not the indices related to the commonly used one. The last group show an amelioration for all the indices.

We have proposed criteria to discriminate the three groups. These criteria where used on a validation cohort to constitute three groups. Their global characteristics were the same as in the original cohort and it comforts the validity of the method. This work will be used by physiologists to propose new criteria for the measure of the effect of a BD treatment. It is in collaboration with physiologists from Bordeaux and Nantes universities and is the object of a paper that will be soon submitted in an international peer-reviewed journal in the domain of pneumology.

6.9. Numerical computation of expectations of PDMP’s

Participants: Adrien Brandejsky, Benoît de Saporta, François Dufour.

This work concerns the computation of expectations of functionals of piecewise deterministic Markov processes (PDMP’s). We propose a numerical scheme to approximate such expectations, analyze the convergence of our scheme and derive bounds for the convergence rate. More precisely, we are interested in the approximation of expectations of the form

$$E_x \left[ \int_{t=0}^{T_n} l(X_t)dt + \sum_{j=1}^{N} c(X_{T_j^-})I_{\{X_{T_j^-} \in \partial E\}} \right]$$

where $(X_t)_{t \geq 0}$ is a PDMP, $(T_j)$ are its jump times and $l$ and $c$ are some non negative, real-valued, bounded functions. Such expectations are discussed by M.H.A. Davis in [50], chapter 3. They often appear as cost or reward functions in optimization problems. The first term is referred to as the running cost while the second may be called the boundary jump cost. Besides, they are quite general since M.H.A. Davis shows how a wide variety of apparently different functionals can be obtained from the above specific form. For example, this wide variety includes quantities such as a mean exit time and even, for any fixed $t \geq 0$, the distribution of $X_t$ (i.e. $E_x[I_{F}(X_t)]$) where $F$ is a measurable set).

There are surprisingly few works in the literature devoted to the actual computation of such expectations, using other means than direct Monte Carlo simulations. M.H.A Davis showed that these expectations satisfy integro-differential equations. However, the set of partial differential equations that is obtained is unusual. Roughly speaking, these differential equations are basically transport equations with a non-constant velocity and they are coupled by the boundary conditions and by some integral terms involving kernels that are derived from the properties of the underlying stochastic process. This approach is currently under study in this project by LATP.

The main difficulty comes from the fact that the domains on which the equations have to be solved vary from one equation to another making their numerical resolution highly problem specific. Another similar approach has been recently investigated in [49], [54]. It is based on a discretization of the Chapman Kolmogorov equations satisfied by the distribution of the process $(X_t)_{t \geq 0}$. The authors propose an approximation of such expectations based on finite volume methods. Unfortunately, their method is only valid if there are no jumps at the boundary.

Our approach is completely different and does not rely on differential equations, but on the fact that such expectations can be computed by iterating an integral operator $G$. This operator only involves the embedded Markov chain $(Z_n, S_n)_{n \in \mathbb{N}}$ and conditional expectations. It is therefore natural to propose a computational method based on the quantization of this Markov chain, following the same idea as [8]. We also addressed two important aspects that had not been investigated in [8]. The first one consists in allowing $c$ and $l$ to be time depending functions, although still Lipschitz continuous, so that we may compute expectations of the form
This important generalization has huge applicative consequences. For instance, it allows discounted cost or reward functions such as \( l(x, t) = e^{-\delta t} l(x) \) and \( c(x, t) = e^{-\delta t} c(x) \) where \( \delta \) is some interest rate. To compute the above expectation, our strategy consists in considering, as it is suggested by M.H.A. Davis in [50], the time augmented process \( \tilde{X}_t = (X_t, t) \).

The second important generalization is to consider the deterministic time horizon problem. Indeed, it seems crucial, regarding to the applications, to be able to approximate

\[
E_x \left[ \int_0^{T_N} l(X_t, t)dt + \sum_{j=1}^{N} c(X_{T_j}, T_j) I\{X_{T_j} \in \partial E\} \right].
\]

for some fixed \( t_f > 0 \) regardless of how many jumps occur before this deterministic time. To compute this quantity, we start by choosing a time \( N \) such that \( P(T_N < t_f) \) be small so that the previous expectation boils down to

\[
E_x \left[ \int_0^{t_f} l(X_t, t)dt + \sum_{j=1}^{N} c(X_{T_j}, T_j) I\{X_{T_j} \in \partial E\} I\{T_j \leq t_f\} \right].
\]

An important advantage of our method is that it is flexible. Indeed, as pointed out in [47], a quantization based method is obstacle free which means, in our case, that it produces, once and for all, a discretization of the process independently of the functions \( l \) and \( c \) since the quantization grids merely depend on the dynamics of the process. They are only computed once, stored off-line and may therefore serve many purposes. Once they have been obtained, we are able to approximate very easily and quickly any of the expectations described earlier. This flexibility is definitely an important advantage of our scheme over standard methods such as Monte-Carlo simulations since, with such methods, we would have to run the whole algorithm for each expectation we want to compute.

The theoretical part of this work with rigorous proofs is under review for an international peer-reviewed journal [10]. F. Dufour presented this work in an invited session at an international conference [22].

### 6.10. Optimal stopping under partial observation

**Participants:** Adrien Brandejsky, Benoîte de Saporta, François Dufour.

In continuation of our work on optimal stopping for Piecewise deterministic Markov processes (PDMP’s) [8], we have started investigating the optimal stopping problem when the process is only partially observed. We supposed that the jump times of the process are observed, but the post jump locations are observed through a noise.
The first step is to rewrite the optimal stopping problem for the partially observed PDMP as a totally observed stopping problem for a new Markov chain, obtained by filtering the observation process. Then, one has to study precisely this filter, which is non standard due to the possible jumps of the process. The next step is to derive the dynamic programming equation adapted to our framework. Finally, we propose a numerical method based on quantization to approximate the value function and \( \epsilon \)-stopping times. Track is also kept of the error bounds all through our numerical procedure.

This work is still in progress and should be submitted to an international peer-reviewed journal shortly.

6.11. Efficient simulation of the availability of a feedwater control system

**Participants:** Benoîte de Saporta, François Dufour, Huilong Zhang.

In the reliability modeling of complex control systems, classical methodologies such as even-trees/fault-trees or Petri nets may not represent adequately the dynamic interactions existing between the physical processes (modeled by continuous variables) and the functional and dysfunctional behavior of its components (modeled by discrete variables). This paper proposes a framework for modeling and simulation of a water level control system in the steam generator (SG) in the secondary circuit of a nuclear power plant. A similar benchmark system was described by the U.S. Nuclear Regulatory Commission [46] to compare two approaches to dynamic reliability: DFM (Dynamic Flowgraph Methodology) and Markov/CCMT (Cell-to-Cell Mapping Technique). But the report released by the NRC is not sufficient to reconstruct a realistic model. We have developed a complete benchmark case. The behavioral model of SG is obtained from a linearized model published in 2000 by EDF [55]. Detailed description of the components, failure modes and control laws of the principal components is presented. For modeling the system, we use the piecewise deterministic Markov processes (PDP) framework [50] and for implementation we chose Simulink associated with Stateflow. PDP’s offer a very general modeling framework to deal with dynamic reliability problems; Simulink is a good tool to simulate non linear differential equations and their controller, while Stateflow implementation is appropriate for finite state machine descriptions of different components.

In our benchmark system, four physical processes are considered: feedwater flowrate, steam flow, narrow range water level and wide range water level. A PID controller is used to maintain the water level within limits of set-points. The system is composed of seven components: 1 passive system representing vapor transport system, 3 extraction pumps, 2 feeding turbopumps, and 1 waterflow regulation valve. The functional and dysfunctional behaviors and the failure rates of each component are based on operational experience.

We show that PDP modeling is suitable for dynamic reliability analysis, and that Simulink associated with Stateflow provides an interactive simulator (graphical block diagramming), which makes the simulator scalable. This work is submitted for presentation to an international conference in 2012.

6.12. Orthogonal Rotation in PCAMIX

**Participants:** Marie Chavent, Jérôme Saracco.

The aim of this work is to propose an efficient algorithm for rotation in PCAMIX, a principal component method for a mixture of qualitative and quantitative variables. We give a new presentation of PCAMIX where the principal components and the squared loadings are obtained from a Singular Value Decomposition. The loadings of the quantitative variables and the principal coordinates of the categories of the qualitative variables are also obtained directly. In this context, we propose a computationaly efficient procedure for varimax rotation in PCAMIX and a direct solution for the optimal angle of rotation. A simulation study shows the good computational behavior of the proposed algorithm. An application on a real data set illustrates the interest of using rotation in MCA. All source codes are available in the R package “PCAmixdata”. This work is in revision for publication [45] and has been presented in [36].


**Participants:** Marie Chavent, Jérôme Saracco.
In this work, we consider block-wise evolving data streams. When a semi-parametric regression model involving a common dimension reduction direction $\beta$ is assumed for each block, we propose an adaptive SIR (for sliced inverse regression) estimator of $\beta$. This estimator is faster than usual SIR applied to the union of all the blocks, both from computational complexity and running time points of view. We show the consistency of our estimator at the root-$n$ rate and its asymptotic normality. We also propose an extension of this method to multiple indices model. In simulation studies, we illustrate the good numerical behavior of our estimator. We also provide a graphical tool in order to detect if there exists a drift of the dimension reduction direction or some aberrant blocks of data. We illustrate our approach with various scenarios. We apply this approach on the following real data problem.

As an illustration, we consider a nonlinear inverse problem in remote sensing. The goal is to estimate the physical properties of surface materials on the planet Mars from hyperspectral data. The method is based on the estimation of the functional relationship between some physical parameters $Y$ and observed spectra $X$. For this purpose, a database of synthetic spectra is generated by a physical radiative transfer model. We propose to reduce the high dimension of spectra ($p = 352$ wavelengths) with a regularized version of SIR. The need to regularize SIR in very high dimensions is well-known. In practice, the database of synthetic spectra may be so large that it cannot be stored in a computer memory. Thus, a stream of smaller sub-databases is generated and we apply our “SIR datastream” approach to this context.

This work will be submitted for publication very soon and it has been presented in the international conference [31].

6.14. Classification of EEG data by evolutionary algorithm for the study of vigilance states

Participants: Marie Chavent, Laurent Vézard.

The objective of this work [42] is to predict the state of vigilance of an individual from the study of its brain activity (EEG signals). The variable to predict is binary (alertness "normal" or "relaxed"). EEG of 44 participants in both states (88 records) were collected with a helmet with 58 electrodes. After a pretreatment step and data validation, a test called "test slope" was chosen. The usual methods of supervised classification (k nearest neighbors, binary classification trees, random forests, and discriminant sparse PLS) were used to provide predictions of the state of participants. The test was then refined using a genetic algorithm, which has built a reliable model (average true classification rate by using CART equal to 86.68 $\pm$ 1.87%) and to select an electrode from the initial 58. This work is in collaboration with Pierrick Legrand (EPI Alea) and Frédérique Faïta (EA 487 "Sciences cognitives et facteur humain").

6.15. Comparison of Kernel Density Estimators on Environmental Data with Assumption on Number of Modes

Participants: Jérôme Saracco, Raphaël Coudret.

In this work, we consider valvometric data samples, that is measurements of distances between the two parts of the shell of bivalves. The movements of a few oysters are monitored in different places (like Arcachon Bay or Santander port) by a laboratory called Environnements et Paléoenvironnements Océaniques et Continentaux (EPOC). The aim of these experiments is to determine water quality via the observation of the bivalves behavior. Previous related works have been published on this subject. EPOC team studied this animals in a copper pollution context via investigations using kernels methods. In our study, we consider each day the density of the distance between the two parts of the shell. This density is reasonably assumed to have 2 modes, the first one corresponds to a close status of the shell and the second one to an open status. The study of the evolution of this density along the time provides informations on bivalves behavior. We provide theoretical results on our bandwidth choice with a bounded support kernel and we give a procedure to determine this bandwidth. We also provide asymptotic results for a density kernel estimator with a kernel that has it support on $\mathbb{R}$. We present an extensive simulation study in order to compare numerical performances of various density
estimators based or not on the two modes assumption. From the results obtained from the simulated data, we derive the suitable estimator for our real data application. This work will be submitted for publication very soon and it has been presented in the international conference [37].
6. New Results

6.1. Autonomous Development of Representations

6.1.1. Open-ended bootstrapping of new sensorimotor representations

Participant: Alexander Gepperth.

We have explored a novel approach to the open-ended development of internal representations in autonomous agents, addressing in particular the transfer of knowledge between different modalities or abstraction levels. We propose a self-organized neural learning paradigm termed PROPRE (projection-prediction) that is driven by predictability: competitive advantages are given to those feature-sensitive elements that are inferable from activity in a reference representation, which may be innate or previously formed by learning. For generating and adapting the new induced representations, PROPRE implements a bi-directional interaction of clustering ("projection") and inference ("prediction"), the key ingredient being an easy-to-compute online measure of predictability, by which the projection step is encouraged to favor sensitivity to predictable clusters. We demonstrated the potential of this paradigm by several simulation experiments with synthetic inputs. We showed that induced representations are indeed significantly more sensitive to predictable stimuli, that they are continuously being adapted to changing input statistics and that the behavior under severe resource constraints is favorable.

6.1.2. The contribution of context information to object detection in intelligent vehicles

Participants: Alexander Gepperth, Michael Garcia Ortiz.

In this work package, we explored the potential contribution of multimodal context information to object detection in an "intelligent car". The used car platform incorporates several sophisticated processing subsystems, both for the detection of objects from local visual patterns as well as for the estimation of global scene properties, e.g., the shape of the road area, or the 3D position of the ground plane (sometimes denoted "scene context" or just "context"). Annotated data recorded on this platform is publicly available as the "HRI RoadTraffic" vehicle video dataset, which formed the basis for this investigation.

In order to quantify the contribution of context information, we investigated whether it can be used to infer object identity with little or no reference to local patterns of visual appearance. Using a challenging vehicle detection task based on the "HRI RoadTraffic" dataset, we trained selected algorithms to estimate object identity from context information alone. In the course of our performance evaluations, we also analyzed the effect of typical real-world conditions (added noise, high dimensions, environmental variation) on context model performance.

As a principal result, we showed that the learning of context models is feasible with all tested algorithms, and that object identity can be estimated from context information with similar accuracy as by relying on local pattern recognition methods. We also found that the use of basis function representations (also known as "population codes") allows the simplest (and therefore most efficient) learning methods to perform best in the benchmark, suggesting that the use of context is feasible even in systems operating under strong performance constraints.

6.1.3. Discovering object concept through developmental learning

Participants: Natalia Lyubova, David Filliat.

The goal of this work is to design a visual system for a humanoid robot. Taking inspiration from children's perception and following the principles of developmental robotics, the robot should detect and learn objects from interactions with people and from experiments it performs with objects, avoiding the use of image databases or of a separate training phase. In our model, all knowledge is therefore iteratively acquired from low-level features and builds up hierarchical object models, which are robust to changes in the environment, background and camera motion.
In our scenario, people in front of the robot are supposed to interact with objects to encourage the robot to focus on them. We therefore assume that the robot is attracted by motion and we segment possible objects based on clustering of the optical flow. Additionally, the depth information from a Kinect is used to filter visual input, considering the constraints of the robot’s working area and to refine the object contours obtained from motion segmentation.

The appearance of objects is encoded following the Bag of Visual Words approach with incremental dictionaries. We combine several complementary features to maximize the completeness of the encoded information (SURF descriptor and superpixels with associated colors) and construct pairs and triples of these features to integrate local geometry information. These features make it possible to decide if the current view has been already seen or not. A multi-view object model is then constructed by associating recognized views and views tracked during object motion.

This system is implemented on the iCub humanoid robot, which detects objects in the visual space and characterizes their appearance, their relative position and their occurrence statistics. Ten objects were presented in the current experiment; each of them was manipulated by a person during 1-2 minutes. Once the vocabulary reached a sufficient amount of knowledge, the robot was able to reliably recognize human hands and most of objects.

6.1.4. Scaling-up Knowledge for a Cognizant Robot

Participants: Thomas Degris, Joseph Modayil.

A cognizant robot is a robot with a deep and immediately accessible understanding of its interaction with the environment—an understanding that the robot can use to flexibly adapt to novel situations. Such a robot will need a vast amount of situated, revisable, and expressive knowledge to display flexible intelligent behaviors. Instead of relying on human-provided knowledge, we consider the case where an arbitrary robot can autonomously acquire pertinent knowledge directly from everyday interaction with the environment. We study how existing ideas in reinforcement learning theory can be used to formalize knowledge and use reinforcement learning techniques to enable a robot to maintain and improve its own knowledge. We consider robot performing a continual learning process that scales-up knowledge acquisition to cover a large number of facts, skills and predictions. This knowledge has semantics that are grounded in sensorimotor experience and can then be used for more abstract process such as planning. We see the approach of developing more cognizant robots as a necessary key step towards broadly competent robots.

Paper being published: Scaling-up Knowledge for a Cognizant Robot accepted at Designing Intelligent Robots: Reintegrating AI, AAAI Spring Symposium 2012.

6.1.5. Learning parallel combinations of motor primitives from demonstration and linguistic guidance with non-negative matrix factorization

Participants: Olivier Mangin, Pierre-Yves Oudeyer.

We have elaborated and experimented a novel approach to joint language and motor learning from demonstration. It enables discovery of a dictionary of motor and linguistic primitives, that can be combined in parallel to represent training data as well as novel skills in the form of combinations of known skills. These methods and the results of our experiments participate in addressing two main issues of developmental robotics: 1) symbol grounding for language learning; 2) achieving compositionality in motor-learning from demonstration, which enables re-using knowledge and thus scaling to complex tasks. In particular, we are interested in learning motor primitives active in parallel, a less explored way of combining such primitives. To address these challenges we have explored and studied the use of nonnegative matrix factorization to discover motor primitives from histogram representations of data acquired from real demonstrations of dancing movements. Initial results were presented in [30] and further results are presented in an article under review.


6.2.1. The SAGG-RIAC algorithm: competence based active learning of motor skills

Participants: Adrien Baranès, Pierre-Yves Oudeyer.
We have continued to develop and experiment the Self-Adaptive Goal Generation - Robust Intelligent Adaptive Curiosity (SAGG-RIAC) algorithm as an intrinsically motivated goal exploration mechanism which allows high-dimensional redundant robots with various body schemas to efficiently and actively learn motor skills in their task space. The main idea is to push the robot to perform active babbling in the low-dimensional goal/task space, as opposed to motor babbling in the high-dimensional actuator space (possibly defined with motor primitives), by self-generating goals actively and adaptively in regions of the task space which provide a maximal competence improvement for reaching those goal states. Then, a lower level active motor learning algorithm is used to drive the robot to locally explore how to reach a given self-generated goal. We have conducted systematic experiments with high-dimensional continuous sensorimotor spaces related to different robotic setups such as a highly-redundant robotic arm, a quadruped, and an arm controlling a fishing rod with a flexible wire and show that 1) exploration in the task space can be a lot faster than exploration in the actuator space for learning inverse models in redundant robots; 2) selecting goals based on the maximal improvement heuristics creates developmental trajectories driving the robot to progressively focus on areas of increasing complexity and is statistically significantly more efficient than selecting goals randomly, as well as more efficient than different standard active motor babbling methods. These results were published in [13], [15], [17] and a journal publication is in preparation.

6.2.2. SGIM-D: Bootstrapping Intrinsically Motivated Learning with Human Demonstration

Participants: Mai Nguyen, Pierre-Yves Oudeyer.

We have studied the coupling of internally guided learning and social interaction, and more specifically the improvement owing to demonstrations, of the learning by intrinsic motivation. We have designed Socially Guided Intrinsic Motivation by Demonstration (SGIM-D), an algorithm for learning the mapping between high dimensions in continuous, non-preset, highly redundant environments. We have shown through a robot learning experiment involving a high-dimensional sensorimotor space related to fishing skills that SGIM-D efficiently combines the advantages of social learning and intrinsic motivation to gain a wide repertoire while being specialised in specific subspaces. An article presenting aspects of this work was awarded the second best student paper award in IEEE ICDL/Epirob 2011 [27].

6.2.3. Maturationally-Constrained Competence-Based Intrinsically Motivated Learning

Participants: Adrien Baranès, Pierre-Yves Oudeyer.

We have continued to develop computational models of the coupling of intrinsic motivations and physiological maturational constraints, showing that both mechanisms may have complex bidirectional interactions allowing the active control of the growth of complexity in motor development which directs an efficient learning and exploration process. The coupling relies on the Self-Adaptive Goal Generation - Robust Intelligent Adaptive Curiosity algorithm (SAGG-RIAC) that instantiates an intrinsically motivated goal exploration mechanism for motor learning of inverse models. Then, we have introduced a functional model of maturational constraints inspired by the myelination process in humans, and showed how it can be coupled with the SAGG-RIAC algorithm, forming a new system called McSAGG-RIAC2. We have then conducted systematic experiments to evaluate qualitative and, more importantly, quantitative properties of these systems when applied to the learning of the forward and inverse kinematic of an unknown robotic arm of up to 60 dimensions, the learning of walking in a 12DOF quadruped controlled with 24 dimensions motor synergies, and learning the control of a fishing rod involving a flexible/rope component. These results were published in [13], [15], [17] and a journal publication is in preparation.

6.2.4. Actor-Critic for Parallel Learning

Participants: Thomas Degris, Matha White, Richard Sutton.

Parallel learning is necessary for a robot to learn multiple tasks in parallel while executing a behavior in the environment not necessarily directly related to the tasks to learn. In previous existing work, an interesting class of learning algorithms for control are actor–critic. First, these algorithms can be used with high-dimensional action space. Second, they also sometimes provide computational models for biological decision-making systems. At FLOWERS, we work on new actor–critic algorithms suitable for parallel learning, with
theoretical guarantees, applicable and practical to use with robots, and formulated in the general framework of reinforcement learning.

6.2.5. Curiosity for Parallel Learning of Predictions and Tasks from the Continuous Interaction of a Robot with its Environment

Participants: Thomas Degris, Adam White, Pierre-Yves Oudeyer.

On one hand, a robot needs a wide variety of knowledge to fully interact with its environment. On the other hand, a robot, like humans or animals, can only perform one behavior at a time in the real world to learn this vast amount of knowledge. A solution to scale up learning while keeping the interaction time with the real world realistic is to learn multiple elements of knowledge simultaneously in parallel. The Horde architecture proposes a set of demons each learning about new policies (i.e. skills) and predictions about these skills (i.e. partial models) off-policy simultaneously. The number of demons learning in parallel is limited only by memory and processing power, and not by the fact that there is only one sensorimotor interaction with the environment to learn from. At FLOWERS, we investigate the question of what the behavior policy of the robot should be to speed-up learning of the demons. Our goal is to test if the Horde scales-up to complex humanoid robots and if, driven by intrinsic motivations, it can autonomously learn building blocks of knowledge for future, more complex, behaviors.

6.2.6. Optimal Teaching on Sequential Decision Tasks

Participants: Manuel Lopes, Maya Cakmak.

A helpful teacher can significantly improve the learning rate of an autonomous learning agent. Teaching algorithms have been formally studied within the field of Algorithmic Teaching. These give important insights into how a teacher can select the most informative examples while teaching a new concept. However the field has so far focused purely on classification tasks. In this paper we introduce a novel method for optimally teaching sequential decision tasks. We present an algorithm that automatically selects the set of most informative demonstrations and evaluate it on several navigation tasks. Next, we present a set of human subject studies that investigate the optimality of human teaching in these tasks. We evaluate examples naturally chosen by human teachers and found that humans are generally sub-optimal. Then based on our proposed optimal teaching algorithm we try to elicit better teaching from humans. We do this by explaining the intuition of the teaching algorithm in an informal language prior to the teaching task. We found that this improves the examples elicited from human teachers on all considered tasks. This shows that a simple modification the instructions given to human teachers, has the potential of greatly improving the performance of the agent trained by the human [41].

6.2.7. Inverse Coordinated Reinforcement Learning

Participants: Manuel Lopes, Jonathan Spraul.

Inverse Coordinated Reinforcement Learning

We extended of inverse reinforcement learning to the multi-agent case. Under this formalism a team of agents can learn a task goal, encoded as a reward function, by observing another team executing that task. Our agents behave using local information and limited communication following the coordinated reinforcement learning framework. We show that a team behavior can be learned using this formalism and how well this mechanism can deal with changing initial conditions and number of agents [68].

6.3. Motor Learning and Morphological Computation

6.3.1. Morphological Computation in Acroban the Humanoid: Balance Control and Dynamic Walking

Participants: Olivier Ly, Pierre-Yves Oudeyer, Matthieu Lapeyre, Jérome Béchu, Paul Fudal, Haylee Fogg.
We have continued to elaborate and experiment the humanoid platform Acroban and its use to study various scientific topics. Our goal was to study three main issues: 1) Compliance and semi-passive dynamics in the framework of dynamic walking in humanoid robots and more generally its impact in terms of semi-passive interactive motor primitives and their robustness to unknown external perturbations; 2) the advantage of a bio-inspired multi-articulated vertebral column in the dynamics of these motor primitives; The platform uses mechatronic components that allow us to adjust dynamically the compliance of actuators, which combines with the intrinsic mechanical compliance of the structure due to the use of elastics and springs. We have explored how these capabilities can allow us to enforce morphological computation in the design of robust dynamic locomotion. Compliance also allows us to design semi-passive motor primitives using the torso as a system of accumulation/release of potential/kinetic energy. This is made possible by the combination of adequate morphology and materials, full-body compliance, semi-passive and self-organized stable dynamics, as well as the possibility to experiment new motor primitives by trial-and-error thanks to light-weightedness. These results were presented in [25]. A dedicated web page with videos is available at: http://flowers.inria.fr/acroban.php.

6.3.2. Maturational constraints for motor learning in high-dimensions: the case of biped walking

Participants: Matthieu Lapeyre, Pierre-Yves Oudeyer, Olivier Ly.

We have elaborated and began to experiment a new developmental approach to motor learning in very high-dimensions, applied to learning biped locomotion in humanoid robots. This approach relies on the formal modeling and coupling of several advanced mechanisms inspired from human development for actively controlling the growth of complexity and harnessing the curse of dimensionality: 1) Maturational constraints for the progressive release of new degrees of freedom and progressive increase their explorative ranges; 2) Motor synergies; 3) Morphological computation; 4) Social Guidance. An experimental setup involving a simulated version of the Acroban Humanoid robot, based on the V-REP simulator, has been elaborated, and initial encouraging results were obtained. These results are presented in [23].

6.3.3. Acroban v2: improving morphological computation with dampers

Participant: Olivier Ly.

Theoretical studies and experiments concerning in particular dynamics of passive walkers drove us to design, construct and continue to experiment a new version of Acroban. This new version has two goals both fitting in the study of the impact of morphology in the behaviour of the robot:

- experiment deep structural modifications of the morphology, in order to avoid as much as possible inelastic chocks. Indeed, during the gait, the unstability is mainly due to chop at the landing of the foot.
- improve the global ratio weight/power of the robot in order to get more dynamic movements.

Indeed, this new version uses RX-28 motors which are lighter than the RX-64 motors which are used in the first version of Acroban. The robot is smaller and lighter. First experiments show that the obtained ratio weight/power is better than the first version. Movements of the robot, and in particular amplitude of locomotion movements, are not limited by torque now. Second, we have experimented plastic materials to design the structure in order to makes is naturally flexible comparing to the metal used in the first version. This way, we improve the natural compliance of the robot. Finally, and this is probably the most important change, we used non actuated linear joints in the hip and in the spline. To control these linear joints, instead of servo-motors, we use dampers. This kind of design is new in humanoid robotic. While bringing new control problems (because of the non-controlled joints which makes the robot semi-passive), this design softens chocks in a significant manner. Experiment shows that stability of the whole structure is greatly improved especially during locomotion.

6.4. HRI and Robot Language Teaching

6.4.1. Intuitive and Robust Physical Human-Robot Interaction with Acroban

Participants: Olivier Ly, Pierre-Yves Oudeyer, Pierre Rouanet, Matthieu Lapeyre, Jérome Béchu, Paul Fudal, Haylee Fogg.
We have experimented and shown how the humanoid robot Acroban allows whole-body robust, natural and intuitive physical interaction with both adults and children. These physical human-robot interaction are made possible through the combination of several properties of Acroban: 1) it is whole-body compliant thanks to variable impedance control and also thanks to the use of elastics and springs; 2) it has a bio-inspired vertebral column allowing more flexibility in postural and equilibrium control; 3) it is light-weight; 4) it has simple low-level controllers that leverage the first three properties. Moreover, the capabilities for physical human-robot interaction that we show are not using a model of the human, and in this sense are “model free”: 1) the capability of the robot to keep its equilibrium while being manipulated or pushed by humans is a result of the intrinsic capability of the whole body to absorb unpredicted external perturbations; 2) the capability of leading Acroban by the hand is an emergent human-robot interface made possible by the self-organizing properties of the body and its low-level controllers and was observed a posteriori only after the robot was conceived and without any initial plan to make this possible. Finally, an originality of Acroban is that is is made with relatively low-cost components which lack of precision is counterbalanced with the robustness due to global geometry and compliance. These results were presented in [28]. A dedicated web page with videos is available at: http://flowers.inria.fr/acroban.php.

6.4.2. A Real World User Study of Different Interfaces for Teaching New Visually Grounded Words to a Robot

Participants: Pierre Rouanet, Pierre-Yves Oudeyer, Fabien Danieau, David Filliat.

We have continued to elaborate and experiment an integrated system based on a combination of advanced Human-Robot Interaction, visual perception and machine learning methods that allows non-expert users to intuitively and robustly teach new visually grounded words to robots. This system is based on the state-of-the-art bags of words technique but focuses on different mediator based interfaces that we can propose to the users. Indeed, we argue that by focusing on interaction we could help users to collect good learning examples and thus improve the performance of the overall learning system. We compared four different interfaces and their impact on the overall system through a real world study where we asked participants to show and teach a robot names for five different objects. Three interfaces were based on mediator objects such as an iPhone, a Wiimote and a laser pointer and provided the users with different kinds of feedback of what the robot is perceiving. The fourth interface was gesture based with a Wizard-of-Oz recognition system included in order to compare our mediator interfaces with a more natural interaction. We showed that the interface may indeed strongly impact the quality of the learning examples collected by users, especially for small objects. More precisely, we showed that interfaces such as the iPhone interface do not only give feedback about what the robot is perceiving but also drive users to pay attention to the learning examples they are collecting. Thus, this interface allows non-expert users to intuitively and easily collect almost as good learning examples as expert users trained for this task and aware of the different visual perception and machine learning issues. Finally, we showed that the mediator based interfaces were judged as easier to use than the a priori more natural gestures based interface. This work was presented in [29].

6.4.3. Language Acquisition as a Particular Case of Context-Dependant Motor Skills Acquisition

Participants: Thomas Cederborg, Pierre-Yves Oudeyer.

Imitation learning, or robot programing by demonstration, have made important advances in recent years. We have proposed to extend the usual contexts investigated to also include linguistic expressions. We have proposed a modification to existing algorithms within the imitation learning framework so that they can handle learning from the demonstration of several unlabelled tasks (or motor primitives) without having to inform the imitator of what task is being demonstrated or what the number of tasks is, which then allows directly for relatively complex language learning. A mechanism for detecting wether or not linguistic/speech input is relevant to the task has also been proposed. With these additions it becomes possible to build an imitator that bridges the gap between imitation learning and language learning by being able to learn linguistic expressions using methods from the imitation learning community. In this sense the imitator learns a word by knowing that a certain speech pattern present in the context means that a specific task is to be executed. The imitator is
however not assumed to know that speech is relevant and has to figure this out on its own by looking at the demonstrations. To demonstrate this ability to find the relevance of speech non linguistic tasks are learnt along with linguistic tasks and the imitator has to figure out when speech is relevant (in some tasks speech should be completely ignored and in other tasks the entire policy is determined by speech). A simulated experiment demonstrates that an imitator can indeed find the number of tasks it has been demonstrated, discover what demonstrations are of what task, for which of the tasks speech is relevant and successfully reproduce those tasks. This work is presented in a publication under review.

6.4.4. Robot Learning by Imitation of Internal Cognitive Operations in the Context of Language Acquisition

Participants: Thomas Cederborg, Pierre-Yves Oudeyer.

We have examined the problem of learning socio-linguistic skills through imitation when those skills involve both observable motor patterns and internal unobservable cognitive operations. This approach is framed in a research program trying to investigate novel links between context-dependent motor learning by imitation and language acquisition. More precisely, the paper presents an algorithm for learning how to respond to communicative/linguistic actions of one human, called an interactant, by observing how another human, called a demonstrator, responds. The response of the demonstrator, which depends on the context, including the signs of the interactant, is assumed to be appropriate and the robotic imitator uses these observations to build a general policy of how to respond to interactant actions. In this paper the communicative actions of the interactant is hand signs, and the learnt behavior consists of how to respond to the hand signs of a small and simple sign language, both in terms of adequately focusing attention on the right part of the scene, and in terms of responding physically. As a response to two continuous signs of the interactant, the demonstrator focuses on one out of three objects, and then performs a movement in relation to the object focused on. An algorithm is proposed based on a similarity metric between demonstrations, and a simulated experiment is presented where the unseen “focus on object” operation and the hand movements are successfully imitated, including in situations where there are no demonstrations. This work has been published in [21].

6.4.5. Learning Simultaneously New Tasks and Feedback Models in Socially Guided Robot Learning

Participants: Manuel Lopes, Thomas Cederborg, Pierre-Yves Oudeyer.

We have developped a system that allows a robot to learn simultaneously new tasks and feedback models from ambiguous feedback in the context of robot learning by imitation. We have considered an inverse reinforcement learner that receives feedback from a user with an unknown and noisy protocol. The system needs to estimate simultaneously what the task is, and how the user is providing the feedback. We have further explored the problem of ambiguous protocols by considering that the words used by the teacher have an unknown relation with the action and meaning expected by the robot. This allows the system to start with a set of known symbols and learn the meaning of new ones. We have presented computational results that show that it is possible to learn the task under a noisy and ambiguous feedback. Using an active learning approach, the system is able to reduce the length of the training period. [24], [26].

6.5. Hardware

6.5.1. Ergo-Robots/FLOWERS Fields: Towards Large-Scale Robot Learning Experiments in the Real World

Participants: Jérome Béchu, Fabien Bénureau, Haylee Fogg, Paul Fudal, Hugo Gimbert, Matthieu Lapeyre, Olivier Ly, Olivier Mangin, Pierre Rouanet, Pierre-Yves Oudeyer.
In the context of its participation to the exhibition “Mathematics: A Beautiful Elsewhere” at Fondation Cartier pour l’Art Contemporain in Paris, starting from 19th October 2011 and to be held until 18th March 2012, the team has elaborated and experimented a robotic experimental set-up called “Ergo-Robots/FLOWERS Fields”. This set-up is not only a way to share our scientific investigations with the general public, but attacks a very important technological challenge impacting the science of developmental robotics: How to design a robot learning experiment that can run continuously and autonomously for several months? Indeed, developmental robotics takes life-long learning and development as one of its central objective and object of study, and thus shall require experimental setups that allow robots to run, learn and develop for extended periods of time. Yet, in practice, this has not been possible so far due to the unavailability of platforms adapted at the same time to learning, exploration, easy and versatile reconfiguration, and extended time of experimentation. Most experiments so far in the field have a duration ranging from a few minutes to a few hours. This is an important obstacle for the progress of developmental robotics, which would need experimental set-ups capable of running for several months. This is exactly the challenge explored by the Ergo-Robots installation, which we have approached by using new generations of affordable yet sophisticated and powerful off-the-shelf servomotors (RX Series from Robotis) combined with an adequately designed software and hardware architecture, as well as processes for streamlined maintenance. The experiment is now running for five months, six days a week, in a public exhibition which has strong constraints over periods of functioning and no continual presence of dedicated technicians/engineers on site. The experiment involves five robots, each with 6 degrees of freedoms, which are endowed with curiosity-driven learning mechanisms allowing them to explore and learn how to manipulate physical objects around them as well as to discover and explore vocal interactions with humans/the visitors. The robots are also playing language games allowing them to invent their own linguistic conventions. A battery of measures has been set up in order to study the evolution of the platform, with the aim of using the results (to be described in an article) as a reference for building future robot learning experiments on extended periods of time, both within the team and in the developmental robotics community. More information available at: http://flowers.inria.fr/ergo-robots.php and http://fondation.cartier.com/.

![Figure 15. Installation of Ergo Robots at Foundation Cartier.](image-url)
GEOSTAT Project-Team

6. New Results

6.1. Multiplicative cascades in real/synthetic oceanographic signals: application to the evaluation of ocean dynamics

Participants: Hussein Yahia, Oriol Pont, Joel Sudre, Véronique Garçon, Claire Pottier [CNES], Antonio Turiel, Christine Provost.

This work is performed during the final year of the HIRESUBCOLOR contract with CNES/NASA. From a fundamental point of view, significant advances have been worked out in the application of complex systems methods for the derivation of new methods for computing ocean dynamics at high spatial resolution (high resolution Sea Surface Temperature, pixel size: 4 x 4 kms). No temporal information is used. Instead, the norms and orientations of low resolution vector fields derived from altimetry and scatterometers are propagated along the scales of turbulent signals. This year, specific study on the propagation of the norm of the vector field has been conducted, resulting in the complete mapping (norm and orientation) of ocean dynamics at the high resolution of Sea Surface Temperature data. Validation is performed by comparison with the output of the ROMS 3D simulation model, with excellent results, and buoy validation is under way. H. Yahia has been invited to the AGU (American Geophysical Union) Fall meeting in San Francisco to make a presentation of HIRESUBCOLOR results (December 5-9 2011) and also to the EGU meeting to be held in Vienna in 2012. In 2011 the complete method for the determination of ocean dynamics has been finalized and it includes:

- the determination of both norm and orientation of the vector fields,
- the propagation along the scale of both geostrophic and ageostrophic dynamics.

These methods are generic, and can be applied to the determination of high resolution information for ocean/atmosphere interaction. For that matter, the Oceanflux proposal has been submitted and accepted, starting November 1, 2011, and a new proposal called MULTICARO will be submitted to CNES-OSTST.

Related publications: [28], [21].

6.2. Endocardial potential analysis for cardiac arrhythmias

Participants: Oriol Pont, Hussein Yahia, Harish Kumar Goddabanahalli, Michel Haissaguerre, Nicolas Derval, Mélèze Hocini.

Cardiac diseases are the main cause of morbidity and mortality in western countries. Both the pathogenic areas and the evolution of the condition are complex to detect and estimate in the case of arrhythmias, specially in atrial and ventricular fibrillation. In these cases, the dynamics of the cardiac potential behaves chaotically in a highly complex way that challenges its description. Under this context, we are working in the direction of the characterization of the heartbeat dynamics in a model-agnostic way. We have performed analysis of heartbeat dynamics through singularity spectrum, empirical analysis of LPEs for the deart-beat Dynamics, and a novel innovative method to distinguish arrhythmic heartbeat with rhythmic heartbeat has been studied.

Intracardial potential is measured by means of electrode catheters used during the radiofrequency ablation procedure for cases of atrial fibrillation. We have found that in the electric potential signal, a simple fast-changing three-state orientation signal can be sifted from its complex but slow-changing modulation. The fast dynamics experimentally fits a Markovian process which can be described in a simple and compact way and its parameters are robustly estimated. This shows a clear change of signature even with small statistics that can be used to detect transitions in the arrhythmia and identify different regimes in them.

Related publications: [18], [23], [19], [24].
6.3. Phonetic segmentation

Participants: Vahid Khanagha, Joshua Winebarger, Khalid Daoudi, Oriol Pont, Hussein Yahia, Régine André-Obrecht.

Previously we had developed a novel phonetic segmentation method based on Microcanonical Multiscale Formalism (MMF). The algorithm was based on precise computation of Local Predictability Exponents (LPEs) at each point, and then using their integration over time axis (ACC) as a quantitative representative of changes in behavior of distribution of these exponents between neighboring phonemes. The piecewise linear estimation of ACC had provided very good segmentation precision. By performing error analysis of the original algorithm, we proposed a 2-step technique which better exploits LPEs to improve the segmentation accuracy. In the first step, we detect the boundaries of the original signal and of a low-pass filtered version, and we consider the union of all detected boundaries as candidates. In the second step, we use a hypothesis test over the local LPE distribution of the original signal to select the final boundaries. In summary following steps have been taken:

- Detailed error analysis of the original method, which resulted in the realization of the fact that a high-pass filtering can help to detect some of the missed boundaries.
- Development of the hypothesis test method, using the Log Likelihood Ratio Test for final decision over a list of candidates.
- Evaluation of the overall 2-step algorithm on the whole train part of the TIMIT database, to compare with the original method.
- Evaluation on test part of TIMIT database to compare with the state of the art methods.

Related publications: [13], [14].

We continued and improved the adaptation of speaker segmentation methods to develop new (nonlinear) techniques for phonetic segmentation. We succeeded in proposing simple and efficient new algorithms that outperform existing ones. Even with new approaches, our nonlinear approach was still competitive.

Related publications: [22], [27].

6.4. Optimal wavelets, unpredictable points manifold and the emergence of complexity

Participants: Oriol Pont, Hussein Yahia, Suman Maji.

We have found new theoretical developments that link the optimal wavelet description with the information transfer that characterizes the singularity exponents in complex signals. This fact is particularly relevant when there exists a microcanonical cascade as an effective dynamics for the underlying complex system. The implication of this is that under a multiscale hierarchy, the unpredictable set of a signal can be described in terms of its optimal wavelet coefficients and the multiplicative cascade relations between them, easing the information inference or reconstructability between resolution levels.

A new method for the detection of the unpredictable points manifold has been developed, enhancing previous implementations. The algorithm exploits the basic signal symmetries that can be easily verified and has the advantage of not assuming any underlying model. That work is the result of the collaboration between our team and A. Turiel’s team at Institute of Marine Sciences of Barcelona.

Additionally, we have developed a new algorithm that allows for the first time a very robust detection of the optimal wavelet in 2D signals. The main advantage of this new algorithm is that it optimizes the wavelet shape in a totally unconstrained way, therefore not restricting to specific wavelet families.

Related Publications: [7], [20].

6.5. Discriminative learning for automatic speaker recognition

Participants: Khalid Daoudi, Reda Jourani, Régine André-Obrecht.
Most of the speaker recognition systems rely on generative learning of Gaussian Mixture Models (GMM). During the last decade, discriminative approaches have been an interesting and valuable alternative to address directly the classification problem. For instance, Support Vector Machines (SVM) combined with GMM supervectors are among state-of-the-art approaches in speaker recognition. Recently a new discriminative approach for multiway classification has been proposed, the Large Margin Gaussian mixture models (LM-GMM). These latter methods have the same advantage as SVM in term of the convexity of the optimization problem to solve. However they differ from SVM because they draw nonlinear class boundaries directly in the input space, and thus no kernel trick is required. We continued our work on investigating simplified versions of LM-GMM for speaker recognition that can handle large scale databases. We developed a new and efficient learning algorithm and evaluated it on NIST-SRE data. The results show that this new algorithm not only outperforms both the original LM-GMM and the traditional GMM, but also outperforms state-of-the-art discriminative methods such as GMM-supervectors SVM.

Related Publications: [9], [10], [11], [12], [8].

6.6. A multiscale approach to phase reconstruction for Adaptive Optics

Participants: Suman Kumar Maji, Hussein Yahia, Oriol Pont, Thierry Fusco, Vincent Michau, Joel Sudre.

Atmospheric turbulence in Earth’s atmosphere upper layers plays a fundamental role in limiting the resolution of ground based instruments. These turbulent layers perturbate to a great extent incoming light from outer space. One of the best known solutions to overcome this hurdle is Adaptative Optics (AO). It provides real-time compensation by deforming a mirror through a servo-loop, according to phase measurements provided by a wavefront sensor (WFS). We propose and experiment with a new model for phase reconstruction from an acquired subimage of the perturbated phase: instead of reconstructing the phase gradient using conventional methods of AO, we propagate along the scales phase information, from the low resolution of the WFS to higher resolution, using specific wavelet projections that mimic inference along the scales associated to cascading properties of fully developed turbulence.

Related Publication: [17].

6.7. Reconstruction of Speech signal from its Unpredictable Points Manifold

Participants: Vahid Khanagha, Khalid Daoudi, Oriol Pont, Hussein Yahia.

Local Predictability Exponents (LPEs) can be used to classify a given signal’s samples according to their predictability. In particular, the Unpredictable Points Manifold, the subset of less predictable points can be formed as the ensemble of points having the least value of singularity exponents. We call these exponents the Local Predictability Exponents since they are computed according to a procedure based on the evaluation of the degree of reconstruction at a given point. We demonstrate in the case of Speech signal that LPEs are key quantities related to predictability in the framework of reconstructible systems: it is possible to reconstruct the whole Speech signal by applying a reconstruction kernel to the UPM. This provides a strong indication of the importance of the UPM, already demonstrated for other types of complex signals. Experiments show that a UPM containing a small number of the points provides very good perceptual reconstruction quality. In summary following steps have been taken:

- Using the LPEs to form the UPM for Speech signal and coping with the implementation issues in particular case of Speech signal.
- Successful reconstruction of Speech signal from the UPM. The performance was measured using objective measures of reconstruction quality.
- Detailed study of geometrical implications of the points in UPM, and proposition of a new multiscale measure, to be used in estimation procedure of exponents, which is more appropriate for speech analysis. In fact, the same quality of reconstruction is achieved with a quite smaller UPM.
- Development of a very simple compression algorithm (8-bit differential nonuniform quantizer) which overperforms the traditional DPCM coding method.
6.8. New upwelling indices from complex system methods

Participants: Hussein Yahia, Ayoub Tamim, Khalid Minaoui, Driss Aboutajdine, Véronique Garçon, Joel Sudre.

We started the Volubilis project on the study of upwelling in the Moroccan coast by satellite imaging. A Ph.D. student, Ayoub Tamim, was recruited in January 2011. We organized the kick-off meeting of the project in Rabat from June 6 to June 10 with the presence of all partners (INRIA, LEGOS, FSR and CRTS). A. Tamim implemented a new version of the software CRTS is using to compute an upwelling index. He then joined GEOSTAT (from September 5 to December 15, 2011) where he first constituted a small validation database of SST and Chlorophyll images. He then implemented some algorithms such as Morand index and multiscale entropy. The goal being to define in a first step a coarse segmentation of upwelling regions.

6.9. A detailed analysis of multisensor fusion of moderate resolution imaging spectroradiometer

Participants: Harish Kumar Goddabanahalli, Dharmendra Singh, Hussein Yahia.

Related publication: [ 16 ].
6. New Results

6.1. Algorithms and high-performance solvers

6.1.1. Dense linear algebra solvers for multicore processors accelerated with multiple GPUs

In collaboration with the Inria RUNTIME team and the University of Tennessee, we have designed dense linear algebra solvers that can fully exploit a node composed of a multicore processor accelerated with multiple GPUs. This work has been integrated in the latest release of the MAGMA package (http://icl.cs.utk.edu/magma/).

6.1.2. Hybrid direct/iterative solvers based on algebraic domain decomposition techniques

A first release of the MaPhyS package should be made available early in 2012 thanks to the developments conducted in the last year of the ADT. An approximation of the local Schur complement has been studied that is based on approximated inverse technique. This work is a natural extension of part of the PhD research of Mikko Byckling. Furthermore, during his master internship, Stojce Nakov has investigated the design of a Krylov subspace method, namely the conjugate gradient, on a run-time system in order to best exploit the computing capabilities of many-GPU nodes and manycore systems. In the framework of his starting PhD funded by TOTAL, Stojce Nakov will continue his work to design a new implementation of a hybrid linear solver (see Section 3.3) for heterogeneous manycore platforms.

6.1.3. Resilience in numerical simulations

In his master internship work, Mawussi Zounon investigated recovery strategies for core faults in the framework of parallel preconditioned Krylov solvers. The underlying idea is to recover fault entries of the iterate via interpolation from existing values available on neighbor cores. He will continue this work in the framework of his PhD funded by the ANR-RESCUE. Notice that these activities are also part of our contribution to the G8-ECS (Enabling Climate Simulation at extreme scale).

6.1.4. Full geometric multigrid method for 3D Maxwell equations

In the context of a collaboration with the CEA/CESTA center, Mathieu Chanaud continued his PhD work on a tight combination between multigrid methods and direct methods for the efficient solution of challenging 3D irregular finite element problems arising from the discretization of Maxwell equations. A parallel solver dedicated to the ODYSSEE challenge (electromagnetism) of CEA/CESTA has been implemented and integrated. The novel parallel solver was able to solve a 1.3 billion system given a 20 million unknown problem at the coarsest level. The input mesh defines the coarsest level. This mesh is further refined to defined the grid hierarchy, where matrix free smoothers are considered to reduce the memory consumption.

6.1.5. Scalable numerical schemes for scientific applications

A work is currently carried on with TOTAL (Rached Abdelkhalek PhD). The extraordinary challenge that the oil and gas industry must face for hydrocarbon exploration requires the development of leading edge technologies to recover an accurate representation of the subsurface. Seismic modeling and Reverse Time Migration (RTM) based on the full wave equation discretization, are tools of major importance since they give an accurate representation of complex wave propagation areas. Unfortunately, they are highly compute intensive. The recent development in GPU technologies with unified architecture and general-purpose languages coupled with the high and rapidly increasing performance throughput of these components made General Purpose Processing on Graphics Processing Units an attractive solution to speed up diverse applications. We have designed a fast parallel simulator that solves the acoustic wave equation on a GPU cluster. Solving the acoustic wave equation in an oil exploration industrial context aims at speeding up seismic modeling and Reverse Time Migration. We consider a finite difference approach on a regular mesh, in both
2D and 3D cases. The acoustic wave equation is solved in a constant density or a variable density domain. All the computations are done in single precision, since double precision is not required in our context. We use nvidia CUDA to take advantage of the GPU computational power. We study different implementations and their impact on the application performance. We obtain a speed up of 16 for Reverse Time Migration and up to 43 for the modeling application over a sequential code running on general purpose CPU. The defense of this thesis is planned early 2012.

For the solution of the elastodynamic equation on meshes with local refinments, we are currently collaborating with Total to design a parallel implementation of a local time refinement technique on top of a discontinuous Galerkin space discretization. This latter technique enables to manage non-conforming meshes suited to deal with multiblock approaches that capture the locally refined regions. this work is developed in the framework of Yohann Dudouit PhD thesis. A software prototype is currently developed to address these simulations.

The calculation of acoustic modes in combustion chambers is a challenging calculation for large 3D geometries. It requires the calculation of a few of the smallest eigenpairs of large unsymmetric matrices in a parallel environment. A new block Arnoldi approach is currently developed to best benefit from the continuation scheme used in this application context. This is part of the PhD research activity of Pablo Salas.

6.2. Efficient algorithmics for code coupling in complex simulations

The performance of the coupled codes depends on how the data are well distributed on the processors. Generally, the data distributions of each code are built independently from each other to obtain the best load-balancing. But once the codes are coupled, the naive use of these decompositions can lead to important imbalance in the coupling area. Therefore, the modeling of the whole coupling is crucial to improve the performance and to ensure a good scalability. The goal is to find the best data distribution for the whole coupled codes and not only for each standalone code. The key idea is to use a graph/hypergraph model that will incorporate information about the coupling itself. Then, we propose new algorithms to perform a coupling-aware partitioning in order to improve the load-balancing of the whole coupled simulation.

Let us consider two coupled codes, modeled by two graphs (or hypergraphs) \( A \) and \( B \), connected by inter-edges \( I(A,B) \) that represents the coupling communications between codes. Formally, the problem consists in partitioning \( A \) in \( M \) and \( B \) in \( N \) with accounting for \( I(A,B) \). This algorithm should optimize both the edge cut for each graph and the coupling communications while maintaining each graph balance. Our general strategy is divided in three main steps:

1. first, we freely partition \( A \) in \( M \) to obtain the partition \( A/M \);
2. then, we projects this partition to \( B \) according to \( I(A,B) \), that provides the partition \( B/M \);
3. finally, we compute the partition \( B/N \) by repartitioning \( B \) from \( M \) existing parts into \( N \).

The final repartitioning step is particularly tedious, because it must handle a variable number of processes. However, as far as we know, the state-of-the-art graph/hypergraph repartitioning tools are limited to a fixed number of processes (i.e. \( M = N \)). To overcome this issue, we have proposed a new repartitioning algorithm – assuming the load is constant – based on hypergraph partitioning technics with fixed vertices. Our algorithm uses an optimal communication pattern, that we have proved to minimize the total number of messages between the former and newer parts. Experimental results validate our work comparing it with other approaches [20]. We currently investigate how to extend our algorithm for the dynamic load-balancing of parallel adaptive codes \( (A = B) \), whose load evolution is variable and difficult to predict. In this case, it would be convenient to dynamically adapt the number of processes used at runtime \( (M \neq N) \), while minimizing migration cost during the repartitioning step. This work is currently conducted in the framework of Clément Vuchener PhD thesis.

6.3. Distributed Shared Memory approach for the steering of parallel simulations
As a different approach of EPSN, we conceived and developed an in-transit visualization framework for interfacing an arbitrary HPC simulation code with an interactive ParaView session using the HDF5 parallel IO library as the API. The library called H5FDdsm is coupled with a ParaView plugin ICARUS (Initialize Compute Analyze Render Update Steer). Because our interface is based on files, stored in a distributed shared memory (DSM), we sought during this year different redistribution strategies to optimize the bandwidth and the transfers between the simulation and the ParaView servers hosting the DSM. This work showed real benefits, particularly on one of our Cray XE6 testing machines using a block cyclic redistribution. On these large HPC machines that do not support the dynamic MPI process management set of functions, we improved our connection system so that simulation and post-processing can be coupled within an MPMD job. Taking also advantage of one-sided communication models and of the Cray Gemini interconnect communication performance, our framework has been sensibly improved and should be optimal in the coming months.

The interface has also been enhanced with a steering interface that allows us to control the simulation workflow and send back not only parameters, but also complete meshes in parallel, which can then be read by the simulation using either our steering interface or HDF5 calls. This has been demonstrated with SPH-flow, a CFD code developed by Ecole Centrale de Nantes and HydrOcean, replacing dynamically and in parallel a falling wedge with a deforming sphere.

This work has been realized and is currently carried on at CSCS - Swiss National Supercomputing Centre in the framework of Jérôme Soumagne PhD thesis (under the co-supervision of Mr. John Biddiscombe) and within the NextMuSE European project 7th FWP/ICT-2007.8.0 ([17], [18], [19]).

6.4. Material physics

6.4.1. Hybrid materials

The study of hybrid materials based on a coupling between molecular dynamics (MD) and quantum mechanism (QM) simulation has been conducted in collaboration with IPREM (Pau) within the ANR CIS 2007 NOSSI (ended December 2011). These simulations are complex and costly and may involve several length scales, quantum effects, components of different kinds (mineral-organic, hydro-philic and -phobic parts). Our goal was to compute dynamical properties of hybrid materials like optical spectra. The computation of optical spectra of molecules and solids is the most consuming time in such coupling. This requires new methods designed for predicting excited states and new algorithms for implementing them. Several tracks have been investigated in the project and new results obtained as described below.

**Optical spectra.**

Some new improvements in our TD-DFT code have been introduced. Our method is based on the LCAO method for densities and excited states that computes electronic excitation spectra. We have worked in two directions:

- As the method introduces a regularization parameter to obtain regularized spectra we have used it to build better algorithms. In particular, we have developed a new hierarchical algorithm that builds a well adapted frequency distribution to better capture the biggest peaks (strongest oscillator strengths) in the spectrum. Moreover, a nonlinear fit method was added and used to compute the transitions and the oscillator strengths of the spectrum.

- In our algorithm, we used a coarse grain paradigm to parallelize the spectrum computation. This approach leads to a memory bottleneck for large systems. In that respect, we have explored a new parallel approach based on a fine grain paradigm (matrix-vector parallelization) to better exploit the manycore architecture of the emerging computers.

Finally, we have improved the packaging of the code to prepare a public release of the code. Our TD-DFT code will be soon available on request.
QM/MM algorithm. For structure studies or dynamical properties, we have coupled QM model based on pseudo-potentials (SIESTA code) with dynamic molecular (DL-POLY code). Therefore we have developed a new algorithm to avoid accounting twice for the forces and the quantum electric field in the molecular model. All algorithms involved in the coupling have been introduced both in SIESTA and in DL-POLY codes. The following new developments needed by the coupling have been introduced in the SIESTA code:

- We have implemented a fast evaluation of the molecular electrostatic field on the quantum grid.
- We have introduced a non periodic Poisson solver based on the parallel linear Hypre solver. This solver allows us to use computation domains as small as possible.
- We have implemented the ElectroStatic Potential (ESP) fit method to obtain more physical point charges than those given by SIESTA with the Mulliken method. These point charges are used by the MM codes to compute electrostatic forces.

Thanks to all our developments introduced in SIESTA a collaboration with the SIESTA research team has started. This enables us to have access to their private svn like repository. Preliminary results on a water dimer and a water box systems show good agreement with other methods developed in SIESTA and DL-POLY teams.

All these results were presented in the final international NOSSI workshop in Biarritz on December.

6.4.2. Material failures

We have started in the context of the OPTIDIS ANR to work on dislocation simulations. The main characteristic of these simulations is that they are highly dynamical. This year, we have started the study of the state of the art on this topic in two directions. The first direction concerns the study of the algorithms used in such simulations and how we can efficiently parallelize them on manycore clusters. In the second one for isotropic materials, we are investigating how to adapt our fast multipole method to compute constraints and then forces in this kind of simulations.
6. New Results

6.1. Modeling

6.1.1. Reassembly

**Participants:** Nicolas Mellado, Patrick Reuter, Gaël Guennebaud, Pascal Barla, Christophe Schlick.

In the context of cultural heritage, 3D laser scanning and photogrammetric 3D acquisition of broken content is becoming increasingly popular, resulting in large collections of detailed fractured archaeological 3D objects that have to be reassembled virtually. We recently investigated a semi-automatic reassembly approach for pairwise matching of digital fragments, that makes it possible to take into account both the archeologist’s expertise, as well as the power of automatic geometry-driven matching algorithms. In order to increase matching efficiency and robustness, we currently focus on shape analysis with higher level representation to guide ICP-like algorithms.

6.2. 3D Data Rendering and Visualization

6.2.1. Soft shadows

**Participant:** Gaël Guennebaud.

Shadows are a fundamental visual effect which both increase the level of realism of a 3D scene, and help to identify spatial relationships between objects. This latter observation makes them particularly important in the context of interactive 3D applications. Generating high quality soft shadows in real-time is still an open challenge. In the continuity of our previous collaboration with the State Key Lab of CAD&CG of Zhejiang University (China) [39], we developed a perceptually based metric dedicated to the prediction of ideal shadow map resolutions [16]. This metric allows us to adaptively generate shadow map tiles. As a result, we managed to render wide and complex exterior scenes with high quality while maintaining high performance (see figure 2).

![Figure 2. Our soft shadow rendering system generates adaptive shadow map tiles and can therefore render softer shadows (right @ 25 fps) faster than their hard shadow counter part (left @ 15 fps).](image)

6.2.2. Synthesis and control of breaking waves

**Participants:** Nicolas Maréchal, Pascal Barla, Gaël Guennebaud, Patrick Reuter.
Modeling complex breaking waves over arbitrary bathymetry is a tedious problem. Currently, most of the existing methods are based on physical simulations by solving the navier-stokes equation. Controlling the shape of breaking waves is almost impossible with such approaches, and the simulation does not run in real-time. In order to overcome these limitations, we propose a phenomenological approach based on a real-time simulation using airy’s wave theory. Our system handles phenomena such as shoaling, refraction and grouping (see figure 3), and the rendering style can be adapted by the user.

Figure 3. Breaking waves generated using our system over an arbitrary bathymetry. 2D wave shape profiles are shown for better legibility.

6.2.3. Analysis and visualization of surface relief

Participants: Lucas Ammann, Pascal Barla, Gaël Guennebaud, Xavier Granier, Patrick Reuter.

Given a base surface with relief, we developed an analysis technique that leverages the complexity found in detailed 3D models for illustrative shading purposes. The key originality of our approach is to extract the relief features such as concavities, convexities and inflections at multiple scales and directions using local cubic-polynomial fitting. We use this information to guide a variety of shading techniques. Our approach is parametrization-free and meshless, allowing for a wide variety of applications ranging from scientific visualization to special effects for the movie industry.

6.3. Expressive Rendering

Figure 4. Conveying visual information through expressive rendering
6.3.1. Line-based Rendering

Participants: Pascal Barla, Jiazhou Chen, Xavier Granier, Christophe Schlick.

We have introduced [18] a new technique called Implicit Brushes to render animated 3D scenes with stylized lines in real-time with temporal coherence. An Implicit Brush is defined at a given pixel by the convolution of a brush footprint along a feature skeleton; the skeleton itself is obtained by locating surface features in the pixel neighborhood. Features are identified via image-space fitting techniques that not only extract their location, but also their profile, which permits to distinguish between sharp and smooth features. Profile parameters are then mapped to stylistic parameters such as brush orientation, size or opacity to give rise to a wide range of line-based styles. This work has won the 3rd best paper award at Eurographics annual conference.

6.3.2. Shape Depiction through Shading

Participants: Pascal Barla, Xavier Granier, Christophe Schlick.

Recently, a number of techniques have been proposed to exaggerate the depiction of shape through the shading of 3D objects. However, existing methods are limited to a single type of material, simple light sources, and they give a fake percept where 3D shape seems to be flattened or embossed, or produce temporal artifacts. We have recently shown that adjusting lighting amplitude for each direction (Radiance Scaling [38], selected as a best paper at I3D 2010 and extended as a TVCG journal paper [17]) may enhance the shape depiction. The technique has been ported to Meshlab (http://meshlab.sourceforge.net/).

6.3.3. Dynamic Expressive Shading Primitives

Participant: Pascal Barla.

Shading appearance in illustrations, comics and graphic novels is designed to convey illumination, material and surface shape characteristics at once. Moreover, shading may vary depending on different configurations of surface distance, lighting, character expressions, timing of the action, to articulate storytelling or draw attention to a part of an object. We have developed [31] a method that imitates such expressive stylized shading techniques in dynamic 3D scenes, and which offers a simple and flexible means for artists to design and tweak the shading appearance and its dynamic behavior. The key contribution of our approach is to seamlessly vary appearance by using a combination of shading primitives that take into account lighting direction, material characteristics and surface features.

6.3.4. Non-Uniform Compositing of Styles

Participants: Jiazhou Chen, Xavier Granier.

In order to investigate how the composition of different styles may help in directing user attention, we have developed [22] a non-uniform composition that integrates multiple rendering styles in a picture driven by an importance map. This map, either issued from salience estimation or designed by a user, is introduced both in the creation of the multiple styles and in the final composition. Our approach accommodates a variety of stylization techniques, such as color desaturation, line drawing, blurring, edge-preserving smoothing and enhancement.

6.4. Interaction

6.4.1. Toucheo: Multitouch + Stereo

Participants: Martin Hachet, Benoit Bossavit, Aurélie Cohé.
We propose a new system that efficiently combines direct multitouch interaction and 3D stereoscopic visualization (see Figure 5). In our approach, the users interact by means of simple 2D gestures on a monoscopic touchscreen, while visualizing occlusion-free 3D stereoscopic objects floating above the surface at an optically correct distance. By coinciding the 3D virtual space with the physical space, we produce a rich seamless workspace where both the advantages of direct and indirect interaction are jointly exploited. In addition to standard multitouch gestures and controls (e.g. pan, zoom, and standard 2D widgets) from which we take advantage, we have designed a dedicated multitouch 3D transformation widget. This widget allows the near-direct control of rotations, scaling, and translations of the manipulated objects. To illustrate the power of our setup, we have designed a demo scenario where participants reassemble 3D virtual fragments. This scenario, as many others, takes benefit of our proposal, where the strength of both multitouch interaction and stereoscopic visualization are unified in an innovative and relevant workspace [19][25]. See highlights.

6.4.2. Touch-based interaction

Participants: Jérémy Laviole, Aurélie Cohé, Martin Hachet.

We have continued exploring 3D User Interfaces for [multi-]touch screens. In particular, in [26], we conducted a user study to better understand the impact of directness on user performance for a RST docking task, for both 2D and 3D visualization conditions. We have also designed a new 3D transformation widget, called tBox, that can be operated easily and efficiently from simple gestures on touch-screens. In our approach, users apply rotations by means of physically plausible gestures, and we have extended successful 2D tactile principles to the context of 3D interaction [23].

6.4.3. Immersive environments

Participant: Martin Hachet.

We have continued working on immersive environments. In particular, with the "Digital Sound" group of LaBRI, we have studied how sound processes should be visualized in immersive setups [13]. Another collaboration is with the REVES Inria project-team, where we have explored how to design 3D pieces of architecture in a CAVE [21].

6.4.4. Brain-Computer Interaction

Participant: Fabien Lotte.

With Fabien Lotte joining the IPARLA team as a research scientist in January 2011, a new research topic related to interaction is being explored: Brain-Computer Interfaces (BCI). BCI are communication systems that enable its users to send commands to the computer by means of brain activity only, this activity being generally measured using ElectroEncephaloGraphy (EEG). This is therefore a new way to interact with computers and interactive 3D applications. In this area, we have explored new techniques to analyze and process EEG signals in order to identify the mental state of the user [14][20]. This has led to improved robustness and mental state recognition performances. Another challenge in BCI is that it requires the collection of several examples.
of EEG signals from the user in order to calibrate the system. This makes the calibration step long and inconvenient. In order to alleviate this problem, we have proposed to generate artificial EEG signals from a few EEG signals already available. Our evaluations have shown that it can indeed significantly reduce the calibration time [28]. Together with the Inria VR4I-team, we have also explored the use of a new mental state to drive a BCI: attention and relaxation states. We have shown that it is indeed possible to identify relaxation and concentration in EEG signals, and that it can be used to drive a BCI [24]. Finally, we have critically analyzed the usefulness and potential of BCI for 3D video games [27].

6.4.5. Tangible user interfaces

**Participant:** Patrick Reuter.

Tangible user interfaces have proven to be useful for the manipulation of 3D objects, such as for selection and navigation tasks, and even for deformation tasks. Deforming 3D models realistically is a crucial task when it comes to study the physical behavior of 3D objects, for example in engineering, in sculpting applications, and in other domains. With recent progress in physical deformation models and the increasing computing power, physically-realistic deformation simulations can now be driven at interactive rates. Consequently, there is an increasing demand for efficient and user-friendly user interfaces for physically-realistic deformation in real-time. We designed a general concept for designing physically-realistic deformations of 3D models with a tangible user interface, and instantiated our concept with a concrete prototype using a passive tangible user interface that incarnates the 3D model and that runs in real-time [32].
6. New Results

6.1. Discrete logarithms

Participant: Andreas Enge.

In [10], we presented for the first time an algorithm for the discrete logarithm problem in certain algebraic curves that runs in subexponential time less than $L(1/2)$, namely, $L(1/3 + \varepsilon)$ for any $\varepsilon > 0$. In [13], we lower this complexity to $L(1/3)$, showing that the corresponding algebraic curves (essentially $C_{ab}$ curves of genus $g$ growing at least quadratically with the logarithmic size of the finite field of definition, $\log q$) result in cryptosystems that are as easily attacked as RSA or traditional cryptosystems based on discrete logarithms in finite fields. We provide a complete classification of all the curves to which the attack applies.

6.2. Class groups and other invariants of number fields

Participants: Jean-François Biasse, Jean-Paul Cerri, Pierre Lezowski.

J.-F. Biasse has determined a class of number fields for which the ideal class group, the regulator, and a system of fundamental units of the maximal order can be computed in subexponential time $L(1/3, O(1))$ (whereas the best previously known algorithms have complexity $L(1/2, O(1))$). This class of number fields is analogous to the class of curves described in [13], cf. ref sec:dlog. The article [18] has been submitted to Mathematics of Computation.

Using new theoretical ideas and his novel algorithmic approach, J.-P. Cerri has discovered examples of generalised Euclidean number fields and of 2-stage norm-Euclidean number fields in degree greater than 2 [11]. These notions, extending the link between usual Euclideanity and principality of the ring of integers of a number field had already received much attention before; however, examples were only known for quadratic fields.

P. Lezowski extended J.-P. Cerri’s algorithm, which was restricted to totally real number fields, to decide whether a generic number field is norm-Euclidean. His procedure allowed to find principal and non norm-Euclidean number fields of various signatures and degrees up to 8, but also to give further insight about the norm-Euclideanity of some cyclotomic fields. Besides, many new examples of generalised Euclidean and 2-stage Euclidean number fields were obtained. The article [25] has been submitted to Mathematics of Computation.

In another direction, norm-Euclidean ideal classes have been studied. They generalise the notion of norm-Euclideanity to non principal number fields. Very few such number fields were known before. A modification of the algorithm provided many new examples and allowed to complete the study of pure cubic fields equipped with a norm-Euclidean ideal class. The article [26] has been submitted to International Journal of Number Theory.

With E. Hallouin, J.-M. Couveignes has studied descent obstructions for varieties [21]. Such obstructions play an important role when one studies families of varieties (e.g. curves of a given genus). Obstructions are often measured by elements in groups like class groups. The theory of stacks provides a more general treatment for these obstructions. Couveignes and Hallouin give the first example of a global obstruction for a variety (that is an obstruction that vanishes locally at every place).

6.3. Number and function field enumeration

Participants: Henri Cohen, Anna Morra, Pieter Rozenhart.
In joint work with R. Scheidler and M. Jacobson, P. Rozenhart has generalized Belabas’s algorithm for tabulating cubic number fields to cubic function fields [30]. This generalization required function field analogues of the Davenport-Heilbronn Theorem and of the reduction theory of binary cubic and quadratic forms. As an additional application, they have modified the tabulation algorithm to compute 3-ranks of quadratic function fields by way of a generalisation of a theorem due to Hasse. The algorithm, whose complexity is quasi-linear in the number of reduced binary cubic forms up to some upper bound $X$, works very well in practice. A follow-up article [29] describes how to use these results to compute 3-ranks of quadratic function fields, in particular yielding examples of unusually high 3-rank.

H. Cohen and A. Morra [12] have obtained an explicit expression for the Dirichlet generating function associated to cubic extensions of an arbitrary number field with a fixed quadratic resolvent. As a corollary, they have proved refinements of Malle’s conjecture in this context.

6.4. Complex multiplication and modularity

Participants: Jean-Marc Couveignes, Andreas Enge, Damien Robert.

The book [16] edited by J.-M. Couveignes and B. Edixhoven, with contributions by J.-M. Couveignes, B. Edixhoven, R. de Jong, F. Merkl and J. Bosman, describes the first polynomial time algorithms for computing Galois representations and coefficients of modular forms. Modular forms are tremendously important in various areas of mathematics, from number theory and algebraic geometry to combinatorics and lattices. Their Fourier coefficients, with Ramanujan’s $\tau$-function as a typical example, have deep arithmetic significance. Prior to this book, the fastest known algorithms for computing these Fourier coefficients took exponential time, except in some special cases. The case of elliptic curves (Schoof’s algorithm) was at the birth of elliptic curve cryptography around 1985. This book gives an algorithm for computing coefficients of modular forms of level one in polynomial time. For example, Ramanujan’s $\tau$ of a prime number $p$ can be computed in time bounded by a fixed power of the logarithm of $p$. Such fast computation of Fourier coefficients is itself based on the main result of the book: the computation, in polynomial time, of Galois representations over finite fields attached to modular forms by the Langlands programme. Because these Galois representations typically have a nonsolvable image, this result is a major step forward from explicit class field theory, and it could be described as the start of the explicit Langlands programme.

The computation of the Galois representations uses their realisation, following Shimura and Deligne, in the torsion subgroup of Jacobian varieties of modular curves. The main challenge is then to perform the necessary computations in time polynomial in the dimension of these highly nonlinear algebraic varieties. Exact computations involving systems of polynomial equations in many variables take exponential time. This is avoided by numerical approximations with a precision that suffices to derive exact results from them. Bounds for the required precision – in other words, bounds for the height of the rational numbers that describe the Galois representation to be computed – are obtained from Arakelov theory. Two types of approximations are treated: one using complex uniformisation and another one using geometry over finite fields.

With F. Morain, A. Enge has determined exhaustively under which conditions “generalised Weber functions”, that is, simple quotients of $\eta$ functions of not necessarily prime transformation level and not necessarily of genus 1, yield class invariants [24]. The result is a new infinite family of generators for ring class fields, usable to determine complex multiplication curves. We examine in detail which lower powers of the functions are applicable, thus saving a factor of up to 12 in the size of the class polynomials, and describe the cases in which the polynomials have integral rational instead of integral quadratic coefficients.

With J.-C. Faugère and D. Lubicz, D. Robert has given an explicit construction for a modular correspondance between abelian varieties [14]. This correspondance describes the algebraic relations of ThetaNullWerte of different levels on isogenous abelian varieties. With R. Cosset, D. Robert has then given an algorithm explaining how to construct the corresponding isogeny, when we are given its (maximally isotropic) kernel [20]. This use a formula by Koizumi for changing the level of the ThetaNullWerte. This is the first algorithm allowing to compute in polynomial time an isogeny between abelian varieties, and a public implementation is available in AVI SOGENIES.
With K. Lauter, D. Robert has worked on improving the computation of class polynomials in genus 2 by the CRT method. This involves some improvements to detect if the curve is maximal, a better sieving of the primes used, and the use of the CRT over the real quadratic field rather than over $\mathbb{Q}$ for the case of dihedral CM fields. The main improvements come from using the above isogeny computation, both in order to be able to find a maximal curve from a curve in the correct isogeny class, and in order to find all others maximal curves from one. A preprint describing these improvements is being written, some details are described in the talk http://www.normalesup.org/~robert/pro/publications/slides/2011-04-C2.pdf.

With Reynald Lercier, J.-M. Couveignes has given in [23] a quasi-linear time randomised algorithm that on input a finite field $\mathbb{F}_q$ with $q$ elements and a positive integer $d$ outputs a degree $d$ irreducible polynomial in $\mathbb{F}_q[x]$. The running time is $d^{1+o(1)} \times (\log q)^{5+o(1)}$ elementary operations. The $o(1)$ in $d^{1+o(1)}$ is a function of $d$ that tends to zero when $d$ tends to infinity. And the $o(1)$ in $(\log q)^{5+o(1)}$ is a function of $q$ that tends to zero when $q$ tends to infinity. The fastest previously known algorithm for this purpose was quadratic in the degree. The algorithm relies on the geometry of elliptic curves over finite fields (complex multiplication) and on a recent algorithm by Kedlaya and Umans for fast composition of polynomials.

### 6.5. Elliptic curve cryptology

**Participants:** Jean-Marc Couveignes, Vincent Verneuil.

In joint work with C. Clavier, B. Feix, G. Gagnerot and M. Roussellet, V. Verneuil has presented in [15] new side-channel analysis results on the AES. They propose improvements on collision-correlation attacks which require less power traces than classical second-order power analysis techniques. In particular, two new methods are presented and are shown to be efficient in practice on two first-order protected AES implementations. They also mention that other symmetric embedded algorithms can be targeted by these new techniques.

With the same coauthors, V. Verneuil has presented new exponentiation algorithms for embedded implementations in [19]. Embedded exponentiation techniques have become a key concern for security and efficiency in hardware devices using public key cryptography. An exponentiation is basically a sequence of multiplications and squarings, but this sequence may reveal exponent bits to an attacker on an unprotected implementation. Although this subject has been covered for years, they present new exponentiation algorithms based on trading multiplications for squarings. This method circumvents attacks aimed at distinguishing squarings from multiplications at a lower cost than other countermeasures. Finally, they present new algorithms using two parallel squaring blocks which provide one of the fastest exponentiation algorithms.

Together with D. Lubicz, D. Robert has extended their algorithm to compute pairings on abelian varieties using theta functions (published at ANTS 2010) to the case of the ate and optimal ate pairings. This involves a description of the Miller functions in term of theta coordinates and an extension of the addition law using more general Riemann relations in order to compute them. The case of theta functions of level 2 has been optimised by introducing a way to compute “compatible” additions without the need for a square roots. A preprint describing these results is being written, and some details can be found in the talk http://www.normalesup.org/~robert/pro/publications/slides/2011-06-Geocrypt.pdf.

With J.-G. Kammerer, J.-M. Couveignes has given in [22] an appropriate geometric method for studying and classifying encodings into elliptic curves in a cryptographic context. Such encodings were first proposed by Icart in 2009, and later on by Farashahi, Kammerer, Lercier, and Renault. But it was a little bit disappointing to see that it was no more than an application of Tartaglia’s result without any geometrical explanations for the existence of such “parameterisations” of elliptic curves. Couveignes and Kammerer have filled this gap by giving exactly what can be expected from geometry: a clear explanation. Moreover, they unify all the recent “parameterisations” of elliptic curves under the same geometric point of view. The approach described in this article uses dual curves with some results coming from intersection theory. The main originality of this work is that these geometrical tools are employed to explain symbolic computations used in cryptography, that is, encoding on elliptic curves.
6. New Results

6.1. Inverse Problems

6.1.1. Reconstruction of an elastic scatterer immersed in a homogeneous fluid

Participants: Hélène Barucq, Rabia Djellouli, Élodie Estecahandy.

The determination of the shape of an obstacle from its effects on known acoustic or electromagnetic waves is an important problem in many technologies such as sonar, radar, geophysical exploration, medical imaging and nondestructive testing. This inverse obstacle problem (IOP) is difficult to solve, especially from a numerical viewpoint, because it is ill-posed and nonlinear. Its investigation requires as a prerequisite the fundamental understanding of the theory for the associated direct scattering problem, and the mastery of the corresponding numerical solution methods.

In this work, we are interested in retrieving the shape of an elastic obstacle from the knowledge of some scattered far-field patterns, and assuming certain characteristics of the surface of the obstacle. The corresponding direct elasto-acoustic scattering problem consists in the scattering of time-harmonic acoustic waves by an elastic obstacle $\Omega_s$ embedded in a homogeneous medium $\Omega_f$, that can be formulated as follows:

$$\Delta p + \left(\frac{\omega^2}{c_f^2}\right)p = 0 \quad \text{in } \Omega_f$$

$$\nabla \cdot \sigma(u) + \omega^2 \rho_s u = 0 \quad \text{in } \Omega_s$$

$$\omega^2 \rho_f u \cdot n = \partial p / \partial n + \partial e^{i(\omega/c_f)}x \cdot d / \partial n \quad \text{on } \Gamma$$

$$\sigma(u)n = -\rho_m e^{i(\omega/c_f)}x \cdot d n \quad \text{on } \Gamma$$

$$\lim_{r \to +\infty} r \left( \partial p / \partial r - i \left( \omega / c_f \right) p \right) = 0$$

(3)

where $p$ is the fluid pressure in $\Omega_f$ whereas $u$ is the displacement field in $\Omega_s$, and $\sigma(u)$ represents the stress tensor of the elastic material.

This boundary value problem has been investigated mathematically and results pertaining to the existence, uniqueness and regularity can be found in [65] and the references therein, among others. We propose a solution methodology based on a regularized Newton-type method for solving the IOP. The proposed method is an extension of the regularized Newton algorithm developed for solving the case where only Helmholtz equation is involved, that is the acoustic case by impenetrable scatterers [55]. The direct elasto-acoustic scattering problem defines an operator $F : \Gamma \rightarrow p_\infty$ which maps the boundary $\Gamma$ of the scatterer $\Omega_s$ onto the far-field pattern $p_\infty$. Hence, given one or several measured far-field patterns $p_\infty(\hat{x})$, corresponding to one or several given directions $d$ and wavenumbers $k$, one can formulate IOPs as follows:

Find a shape $\Gamma$ such that $F(\Gamma)(\hat{x}) = p_\infty(\hat{x}); \quad \hat{x} \in S^1$.

We propose a solution methodology based on a regularized Newton-type method to solve this inverse obstacle problem. At each Newton iteration, we solve the forward problem using a finite element solver based on discontinuous Galerkin approximations, and equipped with high-order absorbing boundary conditions. We have first characterized the Fréchet derivatives of the scattered field. They are solution to the same boundary value problem as the direct problem with other transmission conditions. This work has been presented both in FACM11 and in WAVES 2011. A paper has been submitted.
6.1.2. Seismic data interpretation using the Hough transform and principal component analysis

**Participants:** M.-G Orozco-del-Castillo, Carlos Ortiz-Aleman, Roland Martin, Rafael Avila-Carrera, Alejandro Rodriguez-Castellanos.

In [29], two novel image processing techniques are applied to detect and delineate complex salt bodies from seismic exploration profiles: Hough transform and principal component analysis (PCA). It is well recognized by the geophysical community that the lack of resolution and poor structural identification in seismic data recorded at sub-salt plays represent severe technical and economical problems. Under such circumstances, seismic interpretation based only on the human-eye is inaccurate. Additionally, petroleum field development decisions and production planning depend on good-quality seismic images that generally are not feasible in salt tectonics areas. In spite of this, morphological erosion, region growing and, especially, a generalization of the Hough transform (closely related to the Radon transform) are applied to build parabolic shapes that are useful in the idealization and recognition of salt domes from 2D seismic profiles. In a similar way, PCA is also used to identify shapes associated with complex salt bodies in seismic profiles extracted from 3D seismic data. To show the validity of the new set of seismic results, comparisons between both image processing techniques are exhibited. It is remarkable that the main contribution of this work is oriented in providing the seismic interpreters with new semi-automatic computational tools. The novel image processing approaches presented here may be helpful in the identification of diapirs and other complex geological features from seismic images. Conceivably, in the near future, a new branch of seismic attributes could be recognized by geoscientists and engineers based on the encouraging results reported here.

6.1.3. Gravimetry Inversion

**Participants:** Roland Martin, Dimitri Komatitsch, Mark Jessel, Stéphane Perrouty, Vadim Monteiller.

In order to improve the subsoil images in regions which are not well covered by a dense seismic array or can not be well retrieved by using seismic imaging techniques alone (salty dome regions like in the Gulf of Mexico for instance), we have been developing new gravity imaging techniques using supercomputing. In regions like Ghana or the Chicxulub crater located in Yucatan plate (Mexico), 3D sensitivity kernels are calculated for gravity potential data sets measured over 2000 up to 10000 locations randomly distributed in space. The density anomaly computational domain covers a 250 km × 250 km × 20 km volume in these two regions. For instance for the Ghana region two resolutions are taken: 1 point each 2 kms in the horizontal plane and 200 m in the vertical direction in the less accurate configuration and one point each 500 m in the horizontal plane and one point each 100 m in the vertical direction for the most accurate configuration. The gravity anomalies are inverted using an optimized least-square method applied to a sensitivity kernel of \(10^{10}\) up to \(4 \times 10^{11}\) elements. The least-square method using a \(L^2\)-norm or \(L^1\)-norm has been implemented on hybrid multi-CPU/multi-GPU Titanne machines at CCRT of the French Nuclear Energy Agency. \(L^1\) norm gives us sharper boundaries of the density structures when compared to \(L^2\)-norm solutions but these \(L^1\) solutions are obtained at the expense of one order of magnitude in the number of iterations necessary to the inversion. The \(L^2\)-norm gives slightly smoother solutions but is much more faster than \(L^1\) norm by at least one order of magnitude in terms of acceleration. The optimized CPU version has allowed us to reduce drastically the computation time form 5 hours on 512 processors to 25 minutes. Furthermore the multi-GPU version has decreased this computational time around 15 minutes. Our collaboration with geologists of IRD (Mark Jessell and Stephane Perrouyt) has allowed us to determine a realistic a priori model of Ghana with different resolutions in order to obtain more realistic models after inversion. We are still optimizing the multi-GPU code, with the challenging goal of obtaining results lower than 10 minutes and then obtaining an acceleration factor of at least 4 when compared to the optimized multi-CPU inversion code. By now the code is further optimized and more improvements are already in course in terms of better preconditionning, automatic multi-resolution procedure implementation, gravimetry-seismic joint inversion and extension to the global earth imaging. An international article in a scientific peer-reviewed journal is in preparation.
6.2. Modeling

6.2.1. Local approximate DtN exterior boundary condition
Participants: Hélène Barucq, Rabia Djellouli, Anne-Gaëlle Saint-Guirons.

We investigate analytically the asymptotic behavior of high-order spurious prolate spheroidal modes induced by a second-order local approximate DtN absorbing boundary condition (DtN2) when employed for solving high-frequency acoustic scattering problems. We prove that these reflected modes decay exponentially in the high frequency regime. This theoretical result demonstrates the great potential of the considered absorbing boundary condition for solving efficiently exterior high-frequency Helmholtz problems. In addition, this exponential decay proves the superiority of DtN2 over the widely used Bayliss-Gunzburg-Turkel absorbing boundary condition. This work has been accepted for publication in Progress In Electromagnetics Research B. [19].

6.2.2. Non-reflecting boundary condition on ellipsoidal boundary
Participants: Hélène Barucq, Anne-Gaëlle Saint-Guirons, Sébastien Tordeux.

The modeling of wave propagation problems using finite element methods usually requires the truncation of the computational domain around the scatterer of interest. Absorbing boundary condition are classically considered in order to avoid spurious reflections. In this paper, we investigate some properties of the Dirichlet to Neumann map posed on a spheroidal boundary in the context of the Helmholtz equation. We focus on the impedance coefficients defining the DtN condition and we aim at establishing suitable properties in order to propose an accurate numerical method for their computation. Then, we state the well-posedness of the corresponding mixed problem and propose a variational formulation adapted to a finite element discretization. This work has been submitted.

6.2.3. A new modified equation approach for solving the wave equation
Participants: Cyril Agut, Hélène Barucq, Julien Diaz, Florent Ventimiglia, Roland Martin, Dimitri Komatitsch.

The new method involving $p$-harmonic operator described in section 3.2 has been presented in [13]. We have proved the convergence of the scheme and its stability under a CFL condition. Numerical results in one, two and three-dimensional configurations show that this CFL condition is slightly greater than the CFL condition of the second-order Leap-Frog scheme. We have also studied the penalization parameters involved in the new schemes and their influence of the CFL condition. These results are presented in the PhD thesis of Cyril Agut [11]. In the framework of the PhD thesis of Florent Ventimiglia, we are now considering the extension of this technique to the first order formulation of the elastodynamic equations.

6.2.4. Stability Analysis of an Interior Penalty Discontinuous Galerkin Method for the Wave equation
Participants: Cyril Agut, Hélène Barucq, Julien Diaz.

The Interior Penalty Discontinuous Galerkin Method [42], [38], [61] we use in the IPDG/FEM code requires the introduction of a penalty parameter. Except for regular quadrilateral or cubic meshes, the optimal value of this parameter is not explicitly known. Moreover, the condition number of the resulting stiffness matrix is an increasing function of this parameter, but the precise behaviour has not been explicitied neither. We have carried out a theoretical and numerical study of the CFL condition for quadrilateral and cubic meshes, which is presented in the PhD thesis of Cyril Agut [11]. These results were also presented at the peer-reviewed conference Waves 2011 (Vancouver, Canada, July 2011).

6.2.5. Higher Order Absorbing Boundary Conditions for the Wave Equation
Participants: Hélène Barucq, Julien Diaz, Véronique Duprat.
The numerical simulation of wave propagation is generally performed by truncating the propagation medium. Absorbing boundary conditions are then needed. We construct a new family of absorbing boundary conditions from the factorization of the wave equation formulated as a first order system. Using the method of M.E. Taylor, we show that we can generate an infinite number of boundary conditions which can not be obtained via the Niremberg’s factorization method. The conditions can be applied on arbitrarily-shaped surfaces and involve second-order derivatives. We then propose a reduced formulation of the wave equation using an auxiliary unknown which is defined on the regular surface only. The reduced problem allows one to easily include the boundary conditions inside the variational formulation. The corresponding boundary value problem remains well-posed in suitable Hilbert spaces and we give a demonstration in a framework that is suitable to applications. We then study the long-time behavior of the wave field and we show that it tends to 0 as time tends to infinity. This provides a weak stability result that should be completed in the second part of this work. We have then decided to improve the stability result by performing a quantitative study of the energy. We have then shown that the energy is exponentially decaying if the obstacle is star-shaped and the external boundary is convex. This work has been published as INRIA research Report [34], [35] and two papers are submitted. We have next addressed the issue of enriching these ABCs by representing evanescent and damping waves. This has given rise to a work for the Helmholtz equation and we have shown that the enriched ABCs performed better than standard ABCs. The extension to the acoustic wave has led to new conditions involving fractional derivatives. To the best of our knowledge, it is the first time that fractional derivatives have been used for optimizing the performance of ABCs. These new results have been presented in two seminars (University of Bordeaux I and University of Genova) and in two conferences (FACM11 and WAVES 2011). A paper has been published [17] for the case of evanescent waves and two papers are in preparation. All these results are presented in the PhD thesis of Véronique Duprat [12].

6.2.6. Numerical methods combining local time stepping and mixed hybrid elements for the terrestrial migration

**Participants:** Caroline Baldassari, Hélène Barucq, Henri Calandra [Expert Engineer, TOTAL], Bertrand Denel [Research Engineer, TOTAL], Julien Diaz, Florent Ventimiglia.

In order to justify the use of our code IPDGFEM for the Reverse Time Migration, we have carried out a performance analysis of the Interior Penalty Discontinuous Galerkin method and of the Spectral Element Method. This analysis, which shows that IPDG performs as well as SEM, has been presented in [14].

Another aspect of the work concerns the design of local time-stepping algorithms. The local-time stepping strategy proposed in [5] allows for high-order time schemes where the time scheme is adapted to the various space step of the mesh. However, when the mesh contains both low-order and high-order cells, this method not allows for the adaptation of the order of the time-scheme to the order of the cells. We have then presented a new local time-stepping algorithm where both the order of the scheme and the time step vary in the different parts of the mesh. This method has been presented in [14] and at the peer-reviewed conferences Waves 2011 (Vancouver, Canada, July 2011) and DD20 (Domain Decomposition, San Diego, USA, February 2011).

The local-time stepping algorithm is not adapted to handle dissipation terms. A method has been proposed in [59], but it is based on an Adams-Bashforth scheme and it requires the storage of additional unknowns. We can not use this scheme for the simulation of seismic waves in very large heterogeneous domains due to memory limitation. We are now working on the design of alternative schemes which would not require the introduction of the auxiliary unknowns. This one of the topics of the PhD. thesis of Florent Ventimiglia.

6.2.7. Perfectly Matched Layers for the Shallow Water equations

**Participants:** Hélène Barucq, Julien Diaz, Mounir Tlemcani [Assistant Professor, University of Oran, Algeria].

In [45], we have proposed a new Perfectly Matched Layer for Shallow Water equations. This layer required the computation of an auxiliary variable in the whole computational domain. We are now considering a new strategy, which only requires the computation of the auxiliary variable inside the layer. Moreover, the new methodology seems to be well-adapted to the non-linear shallow water equations. We are now performing numerical tests to confirm this point.
6.2.8. Multiperforated plates in linear acoustics

Participants: Abderrahmane Bendali, M'Barek Fares, Sophie Laurens, Estelle Piot, Sébastien Tordeux.

Acoustic engineers use approximate heuristic models to deal with multiperforated plates in liners and in combustion chambers of turbo-engines. These models were suffering from a lack of mathematical justifications and were consequently difficult to improve. Performing an asymptotic analysis (the small parameter is the radius of the perforations), we have justified these models and proposed some improvement. Our theoretical results have been compared to numerical simulations performed at CERFACS (M’Barek Fares) and to acoustical experiments realized at ONERA (Estelle Piot). Two papers are in preparation.

6.2.9. Asymptotic modeling in electromagnetism

Participants: François Buret, Gabriel Caloz, Monique Dauge, Patrick Dular, Marc Duruflé, Erwan Faou, Laurent Krähenbühl, Victor Péron, Ronan Perrussel, Clair Poignard, Damien Voyer.

The following results rely on several problematics developed in section 3.2, item Asymptotic modeling.

We consider in [21] the equations of electromagnetism set on a domain made of a dielectric and a conductor subdomain in a regime where the conductivity is large. Assuming smoothness for the dielectric–conductor interface, relying on recent works we prove that the solution of the Maxwell equations admits a multiscale asymptotic expansion with profile terms rapidly decaying inside the conductor. This skin effect is measured by introducing a skin depth function that turns out to depend on the mean curvature of the boundary of the conductor. We then confirm these asymptotic results by numerical experiments in various axisymmetric configurations. We also investigate numerically the case of a nonsmooth interface, namely a cylindrical conductor.

We derive new thin layer models in electromagnetism, in [22]. We study the behavior of the electromagnetic field in a biological cell modeled by a medium surrounded by a thin layer and embedded in an ambient medium. We derive approximate transmission conditions in order to replace the membrane by these conditions on the boundary of the interior domain. Our approach is essentially geometric and based on a suitable change of variables in the thin layer. Few notions of differential calculus are given in order to obtain the first-order conditions in a simple way, and numerical simulations validate the theoretical results. Asymptotic transmission conditions at any order are given.

We present a numerical treatment of rounded and sharp corners in the modeling of 2D electrostatic fields in [36]. This work deals with numerical techniques to compute electrostatic fields in devices with rounded corners in 2D situations. The approach leads to the solution of two problems: one on the device where rounded corners are replaced by sharp corners and the other on an unbounded domain representing the shape of the rounded corner after an appropriate rescaling. Both problems are solved using different techniques and numerical results are provided to assess the efficiency and the accuracy of the techniques.

6.2.10. Operator Based Upscaling for Discontinuous Galerkin Methods

Participants: Hélène Barucq, Théophile Chaumont, Julien Diaz, Victor Péron.

Realistic numerical simulations of seismic wave propagation are complicated to handle because they must be performed in strongly heterogeneous media. Two different scales must then be taken into account. Indeed, the medium heterogeneities are very small compared to the characteristic dimensions of the propagation medium. To get accurate numerical solutions, engineers are then forced to use meshes that match the finest scale representing the heterogeneities. Meshing the whole domain with the fine grid leads then to huge linear systems and the computational cost of the numerical method is then very high. It would be thus very interesting to dispose of a numerical method allowing to represent the heterogeneities of the medium accurately while computing on a coarse grid. This is the challenge of multiscale approaches like homogenization or upscaling. In this work, we use an operator-based upscaling method. Operator-based upscaling methods were first developed for elliptic flow problems (see [41]) and then extended to hyperbolic problems (see [62], [73], [72]). Operator-based upscaling method consists in splitting the solution into a coarse and a fine part. The coarse part is defined on a coarse mesh while the fine part is computed on a fine mesh. In order to speed up
calculations, artificial boundary conditions (ABC) are imposed. By enforcing suitable ABCs on the boundary of every cells of the coarse mesh, calculations on the fine grid can be carried out locally. The coarse part is next computed globally on the coarse mesh. Operator-based upscaling methods were so far developed in joint with standard finite element discretisation strategy. In this work, we investigate the idea of combining an operator based upscaling method with discontinuous Galerkin finite element methods (DGFEM). To begin with, we have used the interior penalty method as presented in [42] for elliptic problems and in [61], [60] for the wave equation. This is a quite natural way of addressing this issue because we can use a software package that has been already developed in the team. The first results that we have obtained seem to indicate that an DG operator based upscaling method could be interesting essentially in case of stationary problems. Nevertheless, the numerical analysis of the discretized problem must be continued. This work has been initiated during the internship of Theophile Chaumont-Frelet who was a fourth year engineer student at Rouen INSA. A paper dealing with the case of the Laplace operator will be submitted soon.

6.2.11. Discontinuous Galerkin Methods for Seismic Wave Propagation

**Participants:** Hélène Barucq, Caroline Baldassari, Lionel Boillot, Marie Bonnasse, Julien Diaz, Jérôme Luquel, Vanessa Mattesi, Florent Ventimiglia.

In the framework of our collaboration with Total, we are implementing a Discontinuous Galerkin formulation of the first order elastodynamic wave equations in the platform Diva which is developed by Total. We consider the formulation proposed in [54] for isotropic media. During her post-doc, Caroline Baldassi has implemented a three dimensional code with Perfectly Matched Layers for this formulation. Jérôme Luquel has implemented the 2D version of this code during his internship. In the framework of the internship of Marie Bonnasse and the PhD thesis of Lionel Boillot, we have extended the formulation to Vertical Transverse Isotropic and Tilted Transverse Isotropic media in both 2D and 3D. The introduction of Absorbing Boundary Conditions or of PML is still an open problem for these types of media. It is one of the topics of the PhD thesis of Lionel Boillot.

The version of the code that we are using assumed that the properties of the media (density, velocity,...) are constant on each cells of the mesh. Discontinuous Galerkin methods allow for considering more general configurations, where these properties vary as polynomial functions inside each cells. Hence, it is not necessary to define the interfaces between the different media before constructing the mesh. The discontinuities are taken into account directly inside each cells. Moreover, we are able to consider smoothly varying media. In the framework of the internship of Vanessa Mattesi, we have implemented polynomial velocities in a Discontinuous Galerkin formulation. We have compared the results obtained with this method to the one obtained with piecewise constant properties. We have observed that the new formulation was more accurate and that it allowed for a simpler construction of the mesh. However, these gains do not counterbalance the increase of the computational induced by the new method. We have then concluded that considering piecewise constant properties was more appropriate to model seismic wave propagation.

6.2.12. Elastic surface waves in crystals

**Participants:** José Carcione, Fabio Cavallini, Dimitri Komatitsch, Nathalie Favretto-Cristini.

In [25], we present a review of wave propagation at the surface of anisotropic media (crystal symmetries). The physics for media of cubic and hexagonal symmetries has been extensively studied based on analytical and semi-analytical methods. However, some controversies regarding surfaces waves and the use of different notations for the same modes require a review of the research done and a clarification of the terminology. In a companion paper we obtain the full-wave solution for the wave propagation at the surface of media with arbitrary symmetry (including cubic and hexagonal symmetries) using two spectral numerical modeling algorithms.

In [27], we obtain the full-wave solution for the wave propagation at the surface of anisotropic media using two spectral numerical modeling algorithms. The simulations focus on media of cubic and hexagonal symmetries, for which the physics has been reviewed and clarified in a companion paper. Even in the case of homogeneous media, the solution requires the use of numerical methods because the analytical Green’s
function cannot be obtained in the whole space. The algorithms proposed here allow for a general material variability and the description of arbitrary crystal symmetry at each grid point of the numerical mesh. They are based on high-order spectral approximations of the wave field for computing the spatial derivatives. We test the algorithms by comparison to the analytical solution and obtain the wave field at different faces (stress-free surfaces) of apatite, zinc and copper. Finally, we perform simulations in heterogeneous media, where no analytical solution exists in general, showing that the modeling algorithms can handle large impedance variations at the interface.

6.2.13. Application of an elastoplastic spectral-element method to 3D slope stability analysis

Participants: Hom Nath Gharti, Dimitri Komatitsch, Oye Volker, Roland Martin, Jeroen Tromp.

In [26], we implement a spectral-element method for 3D time-independent elastoplastic problems in geomechanics. As a first application, we use the method for slope stability analyses ranging from small to large scales. The implementation employs an element-by-element preconditioned conjugate gradient solver for efficient storage. The program accommodates material heterogeneity and complex topography. Either simple or complex water table profiles may be used to assess effects of hydrostatic pressure. Both surface loading and pseudostatic seismic loading are implemented. In order to simulate elastoplastic behavior of slopes, a Mohr-Coulomb yield criterion is employed using an initial strain method (i.e., a viscoplastic algorithm). For large-scale problems, the software is parallelized based on domain decomposition using MPI (Message Passing Interface). Strong-scaling measurements demonstrate that the parallelized software performs efficiently. We validate our spectral-element results against several other methods, and apply the technique to simulate failure of an earthen embankment and a mountain slope.

6.2.14. Indirect Boundary Element Method applied to Fluid-Solid Interfaces


In [31], scattering of elastic waves in fluid-solid interfaces is investigated. We use the Indirect Boundary Element Method to study this wave propagation phenomenon in 20 models. Three models are analyzed: a first one with an interface between two half-spaces, one fluid on the top part and the other solid in the bottom; a second model including a fluid half-space above a layered solid; and finally, a third model with a fluid layer bounded by two solid half-spaces. The source, represented by Hankel’s function of the second kind, is always applied in the fluid. This indirect formulation can give to the analyst a deep physical insight on the generated diffracted waves because it is closer to the physical reality and can be regarded as a realization of Huygens’ principle. In any event, mathematically it is fully equivalent to the classical Somigliana’s representation theorem. In order to gauge accuracy we test our method by comparing with an analytical solution known as Discrete Wave Number. A near interface pulse generates scattered waves that can be registered by receivers located in the fluid and it is possible to infer wave velocities of solids. Results are presented in both time and frequency domain, where several aspects related to the different wave types that emerge from this kind of problems are pointed out.

6.2.15. Multiperforated plates in linear acoustics

Participants: Mohamed Amara, Sharang Chaudhry, Julien Diaz, Rabia Djellouli, Magdalena Grigoroscuta-Strugaru.

We have designed a new and efficient solution methodology for solving high-frequency Helmholtz problems. The proposed method is a least-squares based technique that employs variable bases of plane waves at the element level of the domain partition. A local wave tracking strategy is adopted for the selection of the basis at the regional/element level. More specifically, for each element of the mesh partition, a basis of plane waves is chosen so that one of the plane waves in the basis is oriented in the direction of the propagation of the field inside the considered element. The determination of the direction of the field inside the mesh partition is formulated as a minimization problem. Since the problem is nonlinear, we apply Newton’s method to determine the minimum. The computation of Jacobians and Hessians that arise in the iterations of the Newtonâs method is based on the exact characterization of the Fréchet derivatives of the field with
Observation and Modeling for Environmental Sciences - New Results - Project-Team MAGIQUE-3D

6.3. High Performance methods for solving wave equations

6.3.1. Forward and adjoint simulations of seismic wave propagation on fully unstructured hexahedral meshes

Participants: Daniel Peter, Dimitri Komatitsch, Yang Luo, Roland Martin, Nicolas Le Goff, Emanuelle Casarotti, Fery Le Loher, Federica Magnoni, Qinya Liu, Céline Blitz, Tarje Nissen-Meyer, Piero Basini, Jeroen Tromp.

In [30], we present forward and adjoint spectral-element simulations of coupled acoustic and (an)elastic seismic wave propagation on fully unstructured hexahedral meshes. Simulations benefit from recent advances in hexahedral meshing, load balancing and software optimization. Meshing may be accomplished using a mesh generation tool kit such as CUBIT, and load balancing is facilitated by graph partitioning based on the SCOTCH library. Coupling between fluid and solid regions is incorporated in a straightforward fashion using domain decomposition. Topography, bathymetry and Moho undulations may be readily included in the mesh, and physical dispersion and attenuation associated with anelasticity are accounted for using a series of standard linear solids. Finite-frequency Fréchet derivatives are calculated using adjoint methods in both fluid and solid domains. The software is benchmarked for a layercake model. We present various examples of fully unstructured meshes, snapshots of wavefields and finite-frequency kernels generated by Version 2.0 ‘Sesame’ of our widely used open source spectral-element package SPECFEM3D.

6.3.2. Fluid-solid coupling on a cluster of GPU graphics cards for seismic wave propagation

Participant: Dimitri Komatitsch.

In [28], we develop a hybrid multiGPUs and CPUs version of an algorithm to model seismic wave propagation based on the spectral-element method in the case of models of the Earth containing both fluid and solid layers. Thanks to the overlapping of communications between processing nodes on the computer with calculation by means of non-blocking message passing, we obtain excellent weak scalability of this finite-element code on a cluster of 192 GPUs and speedup factors of more than one order of magnitude compared to the same code run on a cluster of traditional CPUs. This enables us to show a new geophysical phenomenon concerning wave propagation of diffracted shear waves in a layer called D” located at the base of the Earth’s mantle, namely that in this layer the transverse and radial components of these waves can undergo a relative shift even in an isotropic Earth model, whereas this observation in real seismological data was interpreted until now as an indication of the presence of anisotropy in this layer.
**MAGNOME Project-Team**

### 6. New Results

#### 6.1. Yeast comparative genomics

**Participants:** David James Sherman, Pascal Durrens [correspondant], Tiphaine Martin, Nicolás Loira.

By using the MAGNOME software developments, including the MAGUS system and YAGA software, we have successfully realized a full annotation and analysis of seven new genomes, provided to the Génolevures Consortium by the CEA–Génoscope (Évry). Two distant genomes from the Debaryomycetaceae and mitosporic Saccharomycetales clades of the Saccharomycetales were annotated using previously published Génolevures genomes [5], [9], [10] as references. A further group of five species, comprised of pathogenic and nonpathogenic species, was analyzed with the goal of identifying virulence determinants[13]. By choosing species that are highly related but which differ in the particular traits that are targeted, in this case pathogenicity, we are able to focus on the few hundred genes related to the trait. The approximately 40,000 new genes from these studies were classified into existing Génolevures families as well as branch-specific families. The results from these two studies will be published in the coming year.

#### 6.2. Assembly, annotation and comparison of Oenococcus strains

**Participants:** David James Sherman, Pascal Durrens, Elisabeth Bon [correspondant], Tiphaine Martin, Aurélie Goulielmakis.

*Oenococcus oeni* is part of the natural microflora of wine and related environments, and is the main agent of the malolactic fermentation (MLF), a step of wine making that generally follows alcoholic fermentation (AF) and contributes to wine deacidification, improvement of sensorial properties and microbial stability. The start, duration and achievement of MLF are unpredictable since they depend both on the wine characteristics and on the properties of the *O. oeni* strains. In collaboration with Patrick Lucas’s lab of the ISVV Bordeaux that is currently proceeding with genome sequencing, explorative and, and comparative genomics, Elisabeth Bon coordinates our efforts into the OENIKITA project (since 2009), a scale switching challenge including highthroughput exploratory and comparative genomics for oenological bacterial starters, and the development of an online web-collaborative multigenomic comparative platform (under development) based on the the Génolevures database architecture and MAGUS / YAGA systems.

**OENI-Genomics axis:** In comparative genomics, we investigated gene repertoire and genomic organization conservation through intra- and inter-species genomic comparisons, which clearly show that the *O. oeni* genome is highly plastic and fast-evolving. Results reveal that the optimal adaptation to wine of a strain mostly depends on the presence of key adaptive loops and polymorphic genes. They also point up the role of horizontal gene transfer and mobile genetic elements in *O. oeni* genome plasticity, and give the first clues of the genetic origin of its oenological aptitudes. As a result of the scaling out challenge, we completed the assembly of 19 fully sequenced *O. oeni* genome variants.

**KITA-Genomics (E. Bon, D. Sherman):** This project that is focused on the sequencing, assembly, exploration and comparison of the *O. kitaharae* genome, has benefited to an international collaboration involving Dr V. Makeev. MAGNOME contributed to the assembly of the genome. The comparison against the *O. oeni* genomic architecture will contribute to shed light on the evolutionary mechanisms which are responsible for the atypically long branch of the genus Oenococcus in phylogenetic trees.
Transcriptomic axis (E. Bon, A. Goulielmakis): Under the supervision of E. Bon, Aurélie Goulielmakis has completed for the ANR DIVOENI a detailed manual annotation of a new reference strain of *O. oeni* and performed comparative transcriptome analysis to identify genes differentially expressed under different culture conditions. We explored and compared how the expression system is solicited when *O. oeni* strains adapted to grow in some niches are placed under stress-exposure conditions. The monitoring of gene expression status between strains, through the definition of a global expression pattern proper to each gene, partially lift the veil on how *O. oeni* genome adapts function to its environment. The weight of genetic background and ecological niche pressure on gene expression flexibility was evaluated, and the *O. oeni* pan-transcriptome architecture characterized. The first guidelines revealed a supra-spatial organization of stress response into activated and repressed larger macro-domains defining functional landmarks and intra-chromosomal territories. Decryption of stress-sensitive gene repertoires promises to be an efficient tool in the conquest of *O. oeni* “domestication” through the identification of molecular markers responsible for different physiological capabilities, and the selection of the best adapted strains.

Gene plasticity modelisation (E. Bon, A. Goulielmakis): A novel axis of research recently emerged under the initiative of E. Bon (pseudOE project) around the detection, characterization and conservation of pseudogenes populations in Oenococcus bacteria. Such topic presents a double interest: phylogenetic at first because it should allow to better estimate the degree of genic/genomic plasticity of these bacteria, and algorithmic then because the pseudogenes are a source of confusion for the automatic prediction of genes. Through a transversal collaboration and a cooperative supervision with the Algorithms for Analysis of Biological Structures Group (P. Ferraro, J. Allali) at LaBRI, Laetitia Bourgeade (PhD, Univ. Bordeaux1) was recruited to develop dedicated methods to improve pseudogenes automatic detection, and therefore gene predictions, and to reconstruct fossil and modern genes evolutionary history.

6.3. Scaling-out

Participants: David James Sherman [correspondant], Pascal Durrens, Tiphaine Martin, Natalia Golenetskaya, Florian Lajus.

The Tsvetok project in MAGNOME targets “scaling out” for data and computation, both to improve capacity for handling large volumes of data and to permit more automatic analysis of projects of the “comparative genomics of related species” type, where a set of genomes is sequenced and analyzed as part of the same process. Natalia Golenetskaya has designed and implemented a NoSQL schema through the identification of standard queries, definition of the appropriate query-oriented storage schema, and mapping of structured values to this schema. This prototype is being tested on an Apache Cassandra ring deployed in MAGNOME’s dedicated computing cluster.

Large-scale data-mining such as that required for comparative genomics is fundamentally *data-parallel*: an initial transformation is applied to every data object of a given type (such as genes or even individual nucleotides), then a statistical machine learning procedure is applied to the transformed data to produce a summary or to learn a classification function. Analyses of this kind are the design goal of the MapReduce paradigm. Using Tsvetok as a generator for Apache Hadoop, Natalia is designing MapReduce solutions for the principal whole-genome and data-mining analyses used by MAGNOME for eukaryote and prokaryote comparative genomics.

6.4. Affinity Proteomics: Standards for affinity binders

Participants: David James Sherman [correspondant], Natalia Golenetskaya.

Last year we successfully completed and released the MIAPAR and PSI-PAR international standards for knowledge representation and data exchange of affinity binder properties, a five-year effort organized as part of the ProteomeBinders and HUPO-PSI consortia. These standards were reported in *Nature Biotechnology* and *Molecular and Cellular Proteomics* to the research community and extend previous work. One long-standing issue is the adoption of these standards by individual researchers in the lab: initial data entry must be simple enough that standards-based reporting can be integrated into the process...
of writing the paper. We used an extensive dataset of affinity proteomics data to evaluate “last mile” tools for data entry and initial reporting of affinity proteomics data, and identified places where existing tools need to be adapted to meet these specific needs[21].

6.5. Inferring metabolic models

Participants: David James Sherman [correspondent], Pascal Durrens, Tiphaine Martin, Nicolás Loira, Anna Zhukova.

In collaboration with Prof Jean-Marc Nicaud’s lab at the INRA Grignon, we developed the first functional genome-scale metabolic model of an oleaginous yeast. Most work in producing genome-scale metabolic models has focused on model organisms, in part due to the cost of obtaining well-annotated genome sequences and sufficiently complete experimental data for refining and verifying the models. However, for many fungal genomes of biotechnological interest, the combination of large-scale sequencing projects and in-depth experimental studies has made it feasible to undertake metabolic network reconstruction for a wider range of organisms.

An excellent representative of this new class of organisms is \textit{Yarrowia lipolytica}, an oleaginous yeast studied experimentally for its role as a food contaminant and its use in bioremediation and cell factory applications. As one of the hemiascomycetous yeasts completely sequenced in the Génolevures program it enjoys a high quality manual annotation by a network of experts. It is also an ideal subject for studying the role of species-specific expansion of paralogous families, a considerable challenge for eukaryotes in genome-scale metabolic construction. To these ends, we undertook a complete reconstruction of the \textit{Y. lipolytica} metabolic network.

Methods: A draft model was extrapolated from the \textit{S. cerevisiae} model iIN800, using \textit{in silico} methods including enzyme conservation predicted using Génolevures and reaction mapping maintaining compartments. This draft was curated by a group of experts in \textit{Y. lipolytica} metabolism, and iteratively improved and validated through comparison with experimental data by flux balance analysis. Gap filling, species-specific reactions, and the addition of compartments with the corresponding transport reactions were among the improvements that most affected accuracy.

Results: We produced an accurate functional model for \textit{Y. lipolytica}, MODEL1111190000 in Biomodels.net, that has been qualitatively validated against gene knockouts.

6.6. Hierarchical modeling with BioRica

Participants: David James Sherman [correspondent], Tiphaine Martin, Alice Garcia, Rodrigo Assar-Cuevas, Nicolás Loira.

A recurring challenge for \textit{in silico} modeling of cell behavior is that experimentally validated models are so focused in scope that it is difficult to repurpose them. Hierarchical modeling 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.

BioRica is a high-level hierarchical modeling framework for models combining continuous and discrete components. By providing a reliable and functional software tool backed by a rigorous semantics, we hope to advance real adoption of hierarchical modeling by the systems biology community. By providing an understandable and mathematically rigorous semantics, this will make is easier for practicing scientists to build practical and functional models of the systems they are studying, and concentrate their efforts on the system rather than on the tool.

Rodrigo Assar formalized two strategies for integrating discrete control with continuous models, coefficient switches that control the parameters of the continuous model, and strong switches that choose different models. This was translated by Alice Garcia into a BioRica specification for hybrid systems that assures integrity of models, allowing composition, reconciliation, and reuse of models with SBML specifications. Rodrigo used this approach to describe two systems: wine fermentation kinetics, and cell fate decisions leading to bone and fat formation[11]. In the first, known models that describe the responses of yeast cells to different
temperatures, resources and toxins, were reconciled using coefficient switches that gave the best adjustment of the model depending on the initial conditions and fermentation variable. In the second, a combination of accurate models to predict the bone and fat formation in response to activation of pathways such as the Wnt pathway, and changes of conditions affecting these functions such as increments in Homocysteine, were used to analyze the responses to treatments for osteoporosis and other bone mass disorders. Our hope is that this is a first step in obtaining \textit{in silico} evaluations of medical treatments before testing them \textit{in vivo} or \textit{in vitro}.

Maria Llubères of the University of Puerto Rico visited MAGNONE and we established formal relationships between BioRica models and probabilistic boolean networks.
6. New Results

6.1. Multi-fluid flows

- Microfluidics: (2011) Participants CHB, Johana Pinilla (doc), Sandra Tancogne (MC Reims) To handle oil recovery by chemical processes it is useful to better understand the behaviour of multi-fluids flows in a saturated soil. The porous medium is mimiced by a network of micro channels. The simulation of immiscible multi-fluids flows is then performed by means of the level-sets and the penalization methods to track the interfaces between the fluids and to get rid of the geometry difficulties. In addition the Cox law is added in the model to better move the interfaces during the simulations.

- Microfluidics: concerning visco-elastic fluids in micro-channel, one has often to compute solutions of system for which the viscosity in the Stokes part is much smaller than that involved in the extra-stress. In his thesis, V. Huber has introduced a new scheme to overcome this difficulties without changing the complexity of the scheme (PhD in progress).

6.2. Cancer modelling

In 2010, we have improved our generic mathematical models describing tumor growth. These models were then specialized for several types of cancer (thyroidal lung nodules, brain tumors). The algorithm used to recover the parameters of these models from medical images has also been greatly improved and is now adapted to run on HPC architectures.

+ Secondary tumors in the lung:
The mathematical models describing the growth of secondary in the lungs have now settled and are well understood. The main focus of the year was to keep on using these models on patient data. New clinical case were selected by clinicians from the Institut Bergonié, there are currently under study. The model is currently able to reproduce the growth observed on 5 clinical cases. In 2011, various improvements to the calibration algorithms were made. The initial seeding of the algorithms was a weak point of the procedure. This has been much improved using a genetic algorithm. A complete rewrite of the routines was done to improve their versatility and efficiency. Previously, the numerical simulations and calibration were performed in 2D (clinicians selected the most relevant slice showing the evolution of the tumor). Work is now ongoing to switch to full 3D computations and calibration.

+ Breast cancer modeling:
In collaboration with the University of Houston and the Methodist Hospital, a new mathematical model describing the growth of breast cancer has been developed. This multi-scale model takes many aspects of the disease into account and allows to study the interplays between the various mechanisms responsible for the evolution of the tumor.

+ Modeling glioblastomas:
In 2011, a hierarchy of models describing the growth of brain tumors was developed (and described in a submitted paper) in collaboration with University of Alabama at Birmingham. As we wished to obtain models that could be calibrated from patient data and yet be reasonably accurate, we believe that these models are suitable trade-offs between the simplicity of the SwansonOs model (the only one used on patient data of brain tumors so far) and the accuracy of more complex models (that cannot really produce quantitative results). In particular, two models were built. The first one allows to study the efficacy of anti-angiogenic therapies. It seems to predict that the efficacy of these treatments is limited, this could be confirmed by a world-wide ongoing clinical study. The second model has been validated and we are trying to recover its parameters for a patient in 3D (which is a rather unique initiative to our knowledge).
+ Modelling of electrochemotherapy: Two articles related to the electrical cell modelling have been done ([58], [54]). The first one deals with the influence of the ionic fluxes on the transmembrane voltage potential and on the cell volume. The main insight of the results consists in linking the transmembrane potential with the cell volume: it has been observed experimentally that cells with a low voltage potential do divide, whereas cells with high voltage potential do not, and the obtained relationship between voltage potential and cell volume can provide an explanation. The second article deals with a new model of cell electroporation essentially based on the experimental results of the I.G.R. In this paper we describe precisely the model, which takes into account the main experimental results in the electroporation process, and we present a variational formulation inherent to the model that leads to new efficient schemes in order to numerically solve the involved P.D.E.

6.3. Newtonian fluid flows simulations and their analysis

- Simulations of water distribution systems: Water losses may constitute a large amount of the distributed total water volume throughout water distribution systems. Here, a new model method is proposed that intends to minimize the total water volume distributed through leakage reduction. Our group has worked on the derivation of advection-reaction-diffusion type equations with an explicit relationship between the local pressure and the leakage rate. An original splitting technique to solve this type of hydraulic problem was then achieved. This technique allows pressure-dependent leakage to be taken into account, whereas in most models leakage is assumed to be uniform along a pipe. Finally, a constrained optimization problem was formulated for leakage reduction in WDS. The control variable had the mean of a local head loss and is considered in the Boundary Conditions to avoid dealing with discontinuities in the governing equations. The objective function to minimize was a regularization of the total water volume distributed. Specific operational constraints were added to ensure enough pressure at consumption points. The direct solution for this minimization problem was sought with a Gradient type method. The leakage reduction was proven to be significant in a case study. The percentage of leakage reduced from 24% to 10% in the linear relationship between pressure and leakage flow rate. With other leakage exponents, the same rate of reduction was achieved. The method was applied on a real network in the South-West of France. Controlling the pressure at two different strategic points permits a significant amount of the total distributed water to be saved (5%). This work was performed in collaboration with Cemagref Bordeaux. Future work will consist of applying a sensibility analysis of control location points to optimize the method.

- Incompressible flows: modeling and simulation of moving and deformable bodies. The incompressible Navier-Stokes equations are discretized in space onto a fixed cartesian mesh. The deformable bodies are taken into using a first order penalization method and/or second order immersed boundary method. The interface between the solid and the fluid is tracked using a level-set description so that it is possible to simulate several bodies freely evolving in the fluid. A turbulence model based on Samgorinsky model has been added to the numerical code. The numerical code written in the C language is massively parallel. The large linear systems (over than 100 millions of dofs) are solved using the Petsc Library. An illustration of the methods, fish-like locomotion is analyzed in terms of propulsion efficiency. Underwater maneuvering and school swimming are also explored. We were able to simulate the three-dimensional flow about a swimmer for realistic physical configurations. See [17]. Another application is the turbulent 3D flow around complex wind turbine (see http://www.math.u-bordeaux1.fr/bergmann/ and http://www.math.u-bordeaux1.fr/MAB/mc2/analysis.html for simulation movies). Wake flows generated by boat propellers are also modeled and simulated.

- Turbulence flow on an hemisphere: (2011) Participants CHB, Patrick Fischer, Yong Liang Xiong (PD) ANR Cyclobulle lead by Hamid Kellay Soap hemi-bubble film experiments have shown some links between the formation of vortices when the hemi-bubble is heated at the equator and the formation of tornados in the earth atmosphere. Two-dimensional simulations using a stereographic map are used to compare to these experimental results and confirm the results when Coriolis force and heat source terms are added.

- Compressible flows: Immersed boundary methods. We are concerned with immersed boundary methods, i.e., integration schemes where the grid does not fit the geometry, and among this class
of methods, more specifically with cartesian grid methods, where the forcing accounting for the presence of boundaries is performed at the discrete level. We have developed a simple globally second order scheme inspired by ghost cell approaches to solve compressible flows, inviscid as well as viscous. In the fluid domain, away from the boundary, we use a classical finite-volume method based on an approximate Riemann solver for the convective fluxes and a centered scheme for the diffusive term. At the cells located on the boundary, we solve an ad hoc Riemann problem taking into account the relevant boundary condition for the convective fluxes by an appropriate definition of the contact discontinuity speed. This method can easily be implemented in existing codes and is suitable for massive parallelization. It has been validated in 1D and 2D for Euler and Navier-Stokes compressible equations. The order of convergence of the method is similar to those observed in the literature: second order globally and first order locally, near the interface for Euler equations, and second order locally and globally for Navier-Stokes equations.

We have developed a new cartesian method to solve elliptic problems with immersed interfaces. These problems appear in numerous applications, among them: heat transfer, electrostatics, fluid dynamics, but also tumour growth modelling, or modelling of electric potential in biological cells. This method is second order accurate in the whole domain, notably near the interface. The originality of the method lies on the use of additional unknowns located on interface points, on which are expressed flux equalities. Special care is dedicated to the discretization near the interface, in order to recover a stable second order accuracy. Actually, a naive discretization could lead to a first order scheme, notably if enough accuracy in the discretization of flux transmission conditions is not provided. Interfaces are represented with a distance level-set function discretized on the grid points. The method has been validated on several test-cases with complex interfaces in 2D. A parallel version has been developed using the PETSC library.

- Simulations of fluid-solid interactions: The interaction of an elastic structure and an fluid occurs in many phenomena in physics. To avoid the difficulty of coupling lagrangian elasticity with an eulerian fluid we consider a whole eulerian formulation. The elasticity of the structure is computed with retrograde characteristics which satisfy a vectorial transport equation. We derive the associated fluid-structure models for incompressible and compressible media. The equations are discretized on a cartesian mesh with finite differences and finite volumes schemes. The applications concern the bio-locomotions and the study of air-elastic interaction.

- Vortex methods: The aim of this work is to couple vortex methods with the penalization methods in order to take advantage from both of them. This immersed boundary approach maintains the efficiency of vortex methods for high Reynolds numbers focusing the computational task on the rotational zones and avoids their lack on the no-slip boundary conditions replacing the vortex sheet method by the penalization of obstacles. This method that is very appropriate for bluff-body flows is validated for the flow around a circular cylinder on a wide range of Reynolds numbers. Its validation is now extended to moving obstacles (axial turbine blades) and three-dimensional bluff-bodies (flow around a sphere). See [71]. Moreover, using the global properties of the penalization method, this technique permits to include porous media simultaneously in the flow computation. We aim to adapt the porous media flows to our new method and to apply it in order to implement passive control techniques using porous layers around bluff-bodies.

- Domain decomposition: Domain decomposition methods are a way to parallelize the computation of numerical solutions to PDE. To be efficient, domain decompositions methods should converge independently on the number of subdomains. The classical convergence result for the additive Schwarz preconditioner with coarse grid is based on a stable decomposition. The result holds for discrete versions of the Schwarz preconditioner, and states that the preconditioned operator has a uniformly bounded condition number that depends only on the number of colors of the domain decomposition, and the ratio between the average diameter of the subdomains and the overlap width. Constants are usually non explicit and are only asserted to depend on the "shape regularity" of the domain decomposition.
Last year, we showed the result holds the additive Schwarz preconditioner can also be defined at the continuous level and provided completely explicit estimates. This year, we established that a similar result also holds for non shape regular domain decompositions where the diameter of the smallest subdomain is significantly smaller than the diameter of the largest subdomain. The constants are also given explicitly and are independent of the ratio between the diameter of the largest subdomain and the diameter of the smallest subdomain.

6.4. Flow control and shape optimization

- Flow control: (2011) Participants CHB, Iraj Mortazavi, Emmanuel Creus (Lille), Patrick Gilliron (Renault chercheur indpendant !) An efficient active control of the two- and three-dimensions flow around the 25¡ rear window Ahmed body has been performed. A careful theoretical and numerical study of the trajectories of the vortices allows to adapt the control in order to improve its efficiency and get a better drag reduction.
6. New Results

6.1. Leveraging Software Architectures to Guide and Verify the Development of Sense/Compute/Control Applications

A software architecture describes the structure of a computing system by specifying software components and their interactions. Mapping a software architecture to an implementation is a well-known challenge. A key element of this mapping is the architecture’s description of the data and control-flow interactions between components. The characterization of these interactions can be rather abstract or very concrete, providing more or less implementation guidance, programming support, and static verification.

In this work, we have introduced a notion of behavioral contract that expresses the set of allowed interactions between components, describing both data and control-flow constraints [15]. This declaration is part of the architecture description, allows generation of extensive programming support, and enables various verifications. We have instantiated our approach in an architecture description language for the domain of Sense/Compute/Control (SCC) applications, and described associated compilation and verification strategies.

The main contributions of this work are the following:

- We have introduced a language for behavioral contracts dedicated to SCC applications.
- We have shown that behavioral contracts can effectively guide the implementation of SCC applications by enabling the generation of highly customized programming frameworks using a dedicated compiler. This approach ensures the conformance between the architecture and the implementation, while facilitating software evolution.
- We have shown that such descriptions are precise enough to verify safety properties such as information flow reachability or behavioral invariants.
- Based on an implementation of behavioral contracts in a design language targeting SCC applications, we have assessed the benefit of behavioral contracts at a conceptual level and in terms of metrics on the resulting code.

6.2. A Step-wise Approach for Integrating QoS throughout Software Development

Non-functional requirements are used to express the quality to be expected from a system. For real-time systems such as avionics, it is critical to guarantee this quality, in particular time-related performance properties. In this domain, deterministic QoS is generally ensured at the execution platform level (e.g., operating systems, distributed systems technologies, hardware specificities), independently of a particular application. When addressing the QoS requirements of a given application, these platform-specific guarantees are not sufficient.

In this work, we have proposed a step-wise QoS approach integrated through all development phases and development artifacts [17]. This approach is dedicated to control-loop systems. Control-loop systems are systems that sense the external environment, compute data, and eventually control the environment accordingly. This kind of systems can be found in a range of domains, including avionics, robotics, and pervasive computing. For example, in the avionics domain, a flight management application is a control-loop system that (1) senses the environment for location and other navigation information, (2) computes the trajectory and (3) modifies the wings configuration accordingly.
The main contributions of this work are the following:

- We have developed a step-wise approach that systematically processes QoS requirements throughout software development. This integrated approach is dedicated to control-loop systems, allowing to rely on a particular architectural pattern and thus enhancing the design and programming support level for non-functional aspects. For now, we focus on time-related performance but the approach could be generalized to other non-functional properties (e.g., CPU or memory consumption).
- Our approach has been integrated into DIASUITE, a tool-based development methodology dedicated to control-loop systems. DIASUITE is based on a dedicated design language that we have enriched with time-related performance properties. This non-functional extension has been used to offer verification and programming support at each development stage.
- Our approach has been applied to the development of avionics applications such as a flight management system and a collision avoidance system. These experiments have demonstrated that our step-wise approach can effectively guide the avionics certification process.

### 6.3. Architecturing Conflict Handling of Pervasive Computing Resources

The rapid development of new devices (further resources) and development tools being opened to third-parties has paved the way to an increasing number of applications being deployed in pervasive computing environments. These applications anarchically access resources. In this situation, it is very common for a resource to be accessed by multiple applications, potentially leading to conflicts. For example, in a building management system, a security application that grants access inside the building, can conflict with an application dealing with emergency situations like fires, preventing the building to be evacuated.

Managing conflicts consists of three main parts, detection, resolution and prevention. These parts crosscut the development cycle of applications and pervasive computing systems. In this work, we have proposed a conflict management process that cleanly separates conflict management tasks by providing a design method and supporting tools [18]. This facilitates the work of developers, architects and administrators, who can follow clear guidelines to manage conflicts.

The main contributions of this work are the following:

- We have identified requirements at different stages during the development cycle that are necessary to detect, resolve, and prevent conflicts. We have assigned duties and responsibilities to existing roles, that are carried out during the conflict management process without interfering with the standard application development.
- We have extended a domain-specific design language to declare conflict resolution at an architectural level. During the conflict management process conditions are specified and prioritized. Afterwards conflicting applications (inter application) or modules (intra application) are linked to these conditions.
- The declared information is used to generate code dedicated to conflict handling. On the one hand, a compiler generates a dedicated framework that guides the implementation of the conflict handling logic at application and system level. On the other hand, it generates code that orchestrates resource accesses and prevents conflicts.
6. New Results

6.1. Theoretical and Methodological Developments

Participants: Cédric Joncour, Andrew Miller, Arnaud Pêcher, Pierre Pesneau, Ruslan Sadykov, Gautier Stauffer, François Vanderbeck.

We made progress in the development of theory and algorithms in the area of “Reformulation and Decomposition Approaches for MIP”, “Mixed Integer Nonlinear Programming”, and “Polyhedral Combinatorics and Graph Theory”.

6.1.1. Column Generation for Extended Formulations

Working in an extended variable space allows one to develop tight reformulations for mixed integer programs. However, the size of the extended formulation grows rapidly too large for a direct treatment by a MIP-solver. Then, one can use projection tools to derive valid inequalities for the original formulation and implement a cutting plane approach. Or, one can approximate the reformulation, using techniques such as variable aggregation or by reformulating a submodel only. Such approaches result in outer approximation of the intended extended formulation. The alternative considered in [28], [25] is an inner approximation obtained by generating dynamically the variables of the extended formulation. It assumes that the extended formulation stems from a decomposition principle: a subproblem admits an extended formulation from which an extended formulation for the original problem can be derived. Then, one can implement column generation for the extended formulation of the original problem by transposing the equivalent procedure for the Dantzig-Wolfe reformulation. Pricing subproblem solutions are expressed in the variables of the extended formulation and added to the current restricted version of the extended formulation along with the subproblem constraints that are active for the subproblem solution.

Our paper [28], [25] revisits the column-and-row generation approach. Our purpose is to show light on this approach, to emphasize its wide applicability, and to present it with a new angle as a method that is natural when considering a problem reformulation based on any extended reformulation of a subproblem, whether it yields the subproblem integer hull or just an approximation of it. In the spirit of [80], column-and-row generation is viewed herein as a generalization of standard column generation, the latter being based on a specific subproblem extended formulation. This generic view not only highlights the scope of applicability of the method, but it also leads to a more general termination condition than the traditional reduced cost criteria and to theoretically stronger dual bounds (observing that solving the integer subproblems yields Lagrangian dual bounds that might be tighter than the extended formulation LP bound). We highlight a key motivation for working in the extended space: there arises natural recombinations of previously generated columns into new subproblem solutions, which results in an acceleration of the convergence. We point out that lifting the master program in the variable space of the extended formulation can be done while carrying pricing in the compact variable space of the original formulation, using any oracle.

With [28], [25], we establish the validity of the column-and-row generation algorithm in a form that encompass all special cases of the literature. The analysis therein should help practitioners to evaluate whether this alternative procedure has potential to outperform classical column generation on a particular problem. Our numerical experiments highlight a key observation: lifting pricing problem solutions in the space of the extended formulation permits their recombination into new subproblem solutions and results in faster convergence.
6.1.2. Primal Heuristics for Branch-and-Price

Our goal is to exploit global optimization decomposition approaches to retrieve very good feasible solution to large scale problem. This required extending primal heuristic paradigms to the context of dynamic generation of the variables of the model. We highlight an important fact: such generic tools typically performs better than problem specific meta-heuristics, in terms of solution quality and computing times. Based on our application specific experience with these techniques [65], [67], [86], [87], and on a review of generic classes of column generation based primal heuristics, in [58], we are developing a full blown review of such techniques, completed with new methods and an extensive numerical study. This research is being carried on in collaboration with the members of the associated team project, SAMBA.

Significant progress has been achieved in developing generic primal heuristics that made their way into commercial mixed integer programming (MIP) solvers. Extensions to the context of a column generation solution approach are considered by our team, in search for generic black-box primal heuristics for use in Branch-and-Price approaches. As the Dantzig-Wolfe reformulation is typically tighter than the original compact formulations, techniques based on rounding its linear programming solution have better chance to yield good primal solutions. The aggregated information built into the column definition and the price coordination mechanism provide a global view at the solution space that may be lacking in somewhat more “myopic” approaches based on compact formulations. However, the dynamic generation of variables requires specific adaptation of heuristic paradigms. We focus on “diving” methods and considered their combination with sub-MIPing, relaxation induced neighborhood search, and truncated backtracking using a Limited Discrepancy Search. These add-ons serves as local-search or diversification/intensification mechanisms. We also consider feasibility pump approaches. The methods are numerically tested on standard models such as Cutting Stock, Vertex Coloring, Generalized Assignment, Lot-Sizing, and Vehicle Routing problems.

6.1.3. Combining Bender’s and Dantzig-Wolfe Decomposition

In the follow-up of [56], [88], [89], [90], we are finalizing our work on the combination of Dantzig-Wolfe and Bender’s decomposition: Bender’s Master is solved by column generation [91]. The application we considered is a multi-layer network design model arising from a real-life telecommunication application where traffic routing decisions imply the installation of expensive nodal equipment. Customer requests come in the form of bandwidth reservations for a given origin destination pair. Bandwidth requirements are expressed as a multiple of nominal granularities. Each request must be single path routed. Grooming several requests on the same wavelength and multiplexing wavelengths in the same optical stream allow the packing of more traffic. However, each addition or withdrawal of a request from a wavelength requires optical to electrical conversion for which a specific portal equipment is needed. The objective is to minimize the number of such equipment. We deal with backbone optical networks, therefore with networks with a moderate number of nodes (14 to 20) but thousands of requests. Further difficulties arise from the symmetries in wavelength assignment and traffic loading. Traditional multi-commodity network flow approaches are not suited for this problem. Four alternative models relying on Dantzig-Wolfe and/or Benders’ decomposition are introduced and compared. The formulations are strengthened using symmetry breaking restrictions, variable domain reduction, zero-one decomposition of integer variables, and cutting planes. The resulting dual bounds are compared to the values of primal solutions obtained through hierarchical optimization and rounding procedures. For realistic size instances, our best approaches provide solutions with optimality gap of approximately 5% on average in around 2 hours of computing time.

6.1.4. Branching in Branch-and-Price: a generic scheme

Our innovative branching scheme, proposed for its compatible with the column generation procedure (it implies no structural modifications to the pricing problem) is now published in Mathematical Programming A [23]. The scheme proceeds by recursively partitioning the sub-problem solution set. Branching constraints are enforced in the pricing problem instead of being dualized in a Lagrangian way. The subproblem problem is solved by a limited number of calls to the provided solver. The scheme avoids the enumeration of symmetric solutions.
6.1.5. Strong Branching Inequalities for Convex Mixed Integer Nonlinear Programs

Strong branching is an effective branching technique that can significantly reduce the size of the branch-and-bound tree for solving Mixed Integer Nonlinear Programming (MINLP) problems. The focus of our paper [24] is to demonstrate how to effectively use discarded information from strong branching to strengthen relaxations of MINLP problems. Valid inequalities such as branching-based linearizations, various forms of disjunctive inequalities, and mixing-type inequalities are all discussed. The inequalities span a spectrum from those that require almost no extra effort to compute to those that require the solution of an additional linear program. In the end, we perform an extensive computational study to measure the impact of each of our proposed techniques. Computational results reveal that existing algorithms can be significantly improved by leveraging the information generated as a byproduct of strong branching in the form of valid inequalities.

6.1.6. Linear and Nonlinear Inequalities for a Nonseparable Quadratic Set

We described some integer-programming based approaches for finding strong inequalities for the convex hull of a quadratic mixed integer nonlinear set containing two integer variables that are linked by linear constraints. This study [31] was motivated by the fact that such sets appear can be defined by a convex quadratic program, and therefore strong inequalities for this set may help to strengthen the formulation of the original problem. Some of the inequalities we define for this set are linear, while others are nonlinear (specifically conic). The techniques used to define strong inequalities include not only ideas related to recent perspective reformulations of MINLPs, but also disjunctive and lifting arguments. Initial computational tests will be presented.

6.1.7. On the composition of convex envelopes for quadrilinear terms

Within the framework of the spatial Branch-and-Bound algorithm for solving Mixed-Integer Nonlinear Programs, different convex relaxations can be obtained for multilinear terms by applying associativity in different ways. The two groupings ((x1x2)x3)x4 and (x1x2x3)x4 of a quadrilinear term, for example, give rise to two different convex relaxations. In previous work, we proved that having fewer groupings of longer terms yields tighter convex relaxations. In this paper [35], we give an alternative proof of the same fact and perform a computational study to assess the impact of the tightened convex relaxation in a spatial Branch-and-Bound setting.

6.1.8. Stable sets in claw-free graphs

A stable set is a set of pairwise non adjacent vertices in a graph and a graph is claw-free when no vertex contains a stable set of size three in its neighborhood. Given weights on the vertices, the stable set problem (a NP-hard problem in general) consists in selecting a set of pairwise non adjacent vertices maximizing the sum of the selected weights. The stable set problem in claw-free graphs is a fundamental generalization of the classic matching problem that was shown to be polynomial by Minty in 1980 (G. Minty. On maximal independent sets of vertices in claw-free graphs. J. Combinatorial Theory B, 28:284-304 (1980)). However, in contrast with matching, the polyhedral structure (i.e. the integer hull of all stable sets in a claw-free graph) is not very well understood and thus providing a ‘decent’ linear description of this polytope has thus been a major open problem in our field.

We proposed a new algorithm to find a maximum weighted stable set in a claw-free graph [45] whose complexity is now drastically better than the original algorithm by Minty (n^4 versus n^0, where n is the number of vertices). We also provided a description of the polyhedra in an extended space (i.e. using additional artificial variables) and an efficient procedure to separate over the polytope in polynomial-time [27]. Beside those main contributions, we published another papers on the strongly minimal facets of the polytope [22].

We also published two survey papers on both the algorithmic and polyhedral aspects of the problem [32], [16].
6.1.9. Chvátal-Gomory rank of 0/1 polytopes

In [17], we study the Chvátal-Gomory rank of 0/1 polytopes. The Chvátal-Gomory procedure is a generic cutting plane procedure to derive the integer hull of polyhedra, and the rank is the number of iterations needed. We revisited a classic framework by Chvátal, Cook and Hartmann (V. Chvátal, W. Cook, and M. Hartmann. On cutting-plane proofs in combinatorial optimization. Linear Algebra and its Applications, 114/115:455-499 (1989)) to prove lower bounds on the CG-rank and we made it more accessible (the original framework was hard to apply). It allowed us to give a very simple construction and to improve the lower bound on the rank of general 0/1 polytopes (the previous weaker lower bound relied on a sophisticated existence theorem by Erdös). This result is important as it shed some new light on a supposedly well understood procedure.

6.1.10. The Circular-Chromatic number

Another central contribution of our team concerns the chromatic number of a graph (the minimum number of independent stable sets needed to cover the graph). We proved that the chromatic number and the clique number of some superfamilies of perfect graphs is computable in polynomial time [19], [18].

We investigated the circular-chromatic number. It is a well-studied refinement of the chromatic number of a graph (designed for problems with periodic solutions): the chromatic number of a graph is the integer ceiling of its circular-chromatic number. Xuding Zhu noticed in 2000 that circular cliques are the relevant circular counterpart of cliques, with respect to the circular chromatic number, thereby introducing circular-perfect graphs, a super-class of perfect graphs.

We proved that the chromatic number of circular-perfect graphs is computable in polynomial time [73], thereby extending Grötschel, Lovász and Schrijver’s result to the whole family of circular-perfect graphs. We gave closed formulas for the Lovász Theta number of circular-cliques (previously, closed formulas were known for circular-cliques with clique number at most 3 only), and derived from them that the circular-chromatic number of circular-perfect graphs is computable in polynomial time [34].

6.2. Model Specific Developments and Applications

Participants: Cédric Joncour, Andrew Miller, Arnaud Pêcher, Pierre Pesneau, Ruslan Sadykov, Gautier Stauffer, Damien Trut, François Vanderbeck.

The models on which we made progress can be partitioned in three areas: “Packing and Covering Problems”, “Network Design and Routing”, and “Planning, Scheduling, and Logistic Problems”.

6.2.1. Bin-Packing and Knapsack with Conflicts

The bin-packing problem consists in finding the minimum number of bin of fixed size one needs to pack a set of items of different sizes. We studied a generalization of this problem where items can be in conflicts and thus cannot be put together in the same bin. We show in [21] that the instances of the literature with 120 to 1000 items can be solved to optimality with a generic Branch-and-Price algorithm, such as our prototype BaPCod, within competitive computing time. Moreover, we solved to optimality all the 37 open instances. The approach involves generic primal heuristics, generic branching, but a specific pricing procedure.

The knapsack variant encountered in our bin packing problem resolution considers conflicts between items. This problem is quite difficult to solve compared to the usual knapsack problem. The latter is already NP-hard, but can be usually efficiently solved by dynamic programming. We have shown that when the conflict graph (the graph defining the conflicts between the items) is an interval graph, this generalization of the knapsack can also be solved quite efficiently by dynamic programming with the same complexity than the one to solve the common knapsack problem. For the case, when the conflict graph is arbitrary, we proposed a very efficient enumeration algorithm which outperforms the approaches used in the literature.
6.2.2. Using graph theory for solving orthogonal knapsack problems

We investigated the orthogonal knapsack problem, with the help of graph theory. The multi-dimensional orthogonal packing problem (OPP) is defined as follows: given a set of items with rectangular shapes, the problem is to decide whether there is a non-overlapping packing of these items in a rectangular bin. The rotation of items is not allowed. A powerful characterization of packing configurations by means of interval graphs was introduced by Fekete and Schepers using an efficient representation of all geometrically symmetric solutions by a so-called packing class involving one interval graph (whose complement admits a transitive orientation: each such orientation of the edges corresponds to a specific placement of the forms) 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.

In [13], [14], [57], we give two new algorithms: the first one is based upon matrices with consecutive ones on each row as data structures and the second one uses so-called MPQ-trees, which were introduced by Korte and Möhring to recognize interval graphs. These two new algorithms are very efficient, as they outperform Fekete and Schepers’ on most standard benchmarks.

6.2.3. Inventory routing and pickup-and-delivery problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. In [15], we considered the planning of single product pickups over time: each site accumulates stock at a deterministic rate; the stock is emptied on each visit. Our objective is to minimize a surrogate measure of routing cost while achieving some form of regional clustering by partitioning the sites between the vehicles. The fleet size is given but can potentially be reduced. Planning consists in assigning customers to vehicles in each time period, but the routing, i.e., the actual sequence in which vehicles visit customers, is considered as an “operational” decision. We developed a truncated branch-and-price algorithm. This exact optimization approach is combined with rounding and local search heuristics to yield both primal solutions and dual bounds that allow us to estimate the deviation from optimality of our solution. We were confronted with the issue of symmetry in time that naturally arises in building a cyclic schedule (cyclic permutations along the time axis define alternative solutions). Central to our approach is a state-space relaxation idea that allows us to avoid this drawback: the symmetry in time is eliminated by modelling an average behavior. Our algorithm provides solutions with reasonable deviation from optimality for large scale problems (260 customer sites, 60 time periods, 10 vehicles) coming from industry. The subproblem is interesting in its own right: it is a multiple-class integer knapsack problem with setups. Items are partitioned into classes whose use implies a setup cost and associated capacity consumption.

Through the internship of Damien Trut, we studied the optimization problem consisted in the planning of the pick-up of full waste container and delivery of empty container at customer sites by simple vehicles that can carry a single container, or vehicles with a trailer attached that have a total capacity of 2 containers but require more time when handling containers. The model is a multi-period, multi-vehicle, pickup and delivery problem, with “many-to-many” multi commodity transfer requirements and transhipment nodes. In its short term variant, urgent order are coming online. We developed the prototype of a branch-and-price approach for this problem. The prototype was used by Exeo to convince their customer of the potential benefit of decision aid tools to automatically generate vehicle routes. Next, we shall be considering the dimensioning of a vehicle fleet and their allocation to cluster of collect points in a periodic solution (for a PhD project).

In collaboration with the group of M-C Speranza of the university of Brescia (Italy), we study the Vehicle Routing Problem with Discrete Split Deliveries (a customer demand can be partition in integer lot assigned to different vehicles). The development is done within BaPCod with specialized pricing and branching scheme.

6.2.4. Time-Dependent Travelling Salesman Problem and Resource Constrained Shortest Path

In [12] we present a new formulation for the Time-Dependent Travelling Salesman Problem (TDTSP). The main feature of our formulation is that it uses, as a subproblem, an exact description of the n-circuit problem. We present a new extended formulation that is based on using, for each node, a stronger subproblem, namely a n-circuit subproblem with the additional constraint that the corresponding node is not repeated in the circuit.
Although the new model has more variables and constraints than the model of Picard and Queyranne (1978), the results given from our computational experiments show that the linear programming relaxation of the new model gives, for many of the instances tested, gaps that are close to zero. We also provided a complete characterization of the feasible set of the corresponding linear programming relaxation in the space of the variables of the PQ model.

Following this work, we proposed an extended formulation in terms of the Asymmetric Travelling Salesman Problem (ATSP) in [33]. A tightening the linear programming relaxation is obtained by i) enhancing the subproblem arising in the standard multicommodity flow (MCF) model for the ATSP and then ii) by using modelling enhancement techniques. We compare the linear programming relaxation of the new formulation with the linear programming relaxation of the three compact and non-dominated formulations presented in Oncan et al. (2009). As a result of this comparison we present an updated classification of formulations for the asymmetric traveling salesman problem (ATSP).

In the intership of André Linhares, we studied the Resource Constrained Shortest Path Problem (RCSPP): we presented some of the state-of-the-art dynamic programming methods for solving the RCSPP in a unified manner, and we proposed some variants of these algorithms. We assessed the effectiveness of these algorithms through computational experiments.

6.2.5. Machine scheduling
The column-and-row generation method presented in [28], [25] is quite effective for the general machine scheduling problem. In our work [29], we show indeed that one of the most efficient approaches to solve this problem is to use time-indexed Integer Programming formulation, and to deal with its huge size by generating variables and constraints dynamically. The numerical results of [29], highlight the significant reduction in computing times that results from applying the column-and-row generation approach.

In [20], we consider the scheduling jobs in parallel, i.e., jobs can be executed on more than one processor at the same time. With the emergence of new production, communication and parallel computing system, the usual scheduling requirement that a job is executed only on one processor has become, in many cases, obsolete and unfounded. In this work, we consider the NP-hard problem of scheduling malleable jobs to minimize the total weighted completion time (or mean weighted flow time). For this problem, we introduce the class of “ascending” schedules in which, for each job, the number of machines assigned to it cannot decrease over time while this job is being processed. We prove that, under a natural assumption on the processing time functions of jobs, the set of ascending schedules is dominant for the problem. This result can be used to reduce the search space while looking for an optimal solution.

6.2.6. One warehouse multi-retailer problem
The One-Warehouse Multi-retailer problem (OWMR) is a very important NP-hard inventory control problem arising in the distribution of goods when one central warehouse is supplying a set of final retailers facing demand from customers. In [30], we provide a simple and fast 2-approximation algorithm for this problem (i.e. an algorithm ensuring a deviation by a factor at most two from the optimal solution). This result is both important in practice and in theory as it allows to approximate large real-world instances of the problem (we implemented this algorithm at IBM and it is within 10% of optimality in practice) and the techniques we developed appear to apply to more general settings. We are extending our results to other inventory control problems.

6.3. Software prototypes, Generic Developments and Specific Tools
Participants: Cédric Joncour, Romain LeGuay, Pierre Pesneau, Ruslan Sadykov, François Vanderbeck.

6.3.1. BaPCod - a generic branch-and-price code
The development of the prototype software platform is now supported by our junior engineer, Romanin Leguay, who started in September. He developed a new interface with the underlying MIP solver allowing multiple solvers to be called in the same run. The svn depository was re-organized in view of the increasing number of users to whom Romain offer precious support. Romain is currently redesigning parts of the code in the perspective of its parallelisation and is doing code profiling to identify bottlenecks.
The software platform BaPCod is continuously improved to include all the methodological features that arise from our research, in particular in our collaborative project with Brazil: SAMBA. BaPCod serves there as a proof-of-concept code and is useful for the transfer of knowledge between the parties, including the company GAPSO (a Brazilian spin-up launched by these academics).

We have two new institutional Beta users: EDF and Paris 6.
RUNTIME Project-Team

6. New Results

6.1. High-Performance Intra-node Collective Operations
Participants: Brice Goglin, Stéphanie Moreaud.

- KNEM is known to improve the performance of point-to-point intra-node MPI communication significantly [60], [18].
- We designed an extended RMA interface in KNEM that suits the needs of point-to-point, collective and RMA operations.
- We showed that the native use of KNEM in MPI collective implementations enabled further optimization by combining the knowledge of collective algorithms with the mastering of KNEM region management and copies [35].
- This work was initiated in the context of our collaboration with the MPICH2 team and is now also pursued within the OPEN MPI project in collaboration with the University of Tennessee in Knoxville.

6.2. I/O-Affinity-aware MPI Communications
Participants: Brice Goglin, Stéphanie Moreaud.

- We demonstrated in the past that the locality of I/O devices within modern computing nodes has the significant impact of the MPI communication performance [11] (Non-Uniform I/O Access, NUIOA).
- A first way to deal with such affinities would be to privilege I/O-intensive processes by placing them near the network interfaces. However, determining the communication-intensiveness may be tricky. Also, some applications have uniform communication patterns. The other way to deal with I/O affinities is to modify the implementation of communication operations given a predetermined task placement.
- We demonstrated that the implementation of collective operations should take I/O affinities into account. Deciding which steps and leaders should be involved in the algorithms based on NUIOA effects led us to improve broadcast performance significantly [34], [18].

6.3. High-Performance Point-to-Point Communications
Participants: Alexandre Denis, Raymond Namyst.

- NEWMADELEINE is our communication library designed for high performance networks in clusters. We have worked on optimizations on low-level protocols so as to improve point-to-point performance.
- We have proposed [29] auto-tuning mechanisms for most parameters of a communication library: rendez-vous threshold, multi-rail ratio, optimization strategies.
- We have proposed a communication protocol [33] for InfiniBand that completely amortizes the cost of memory registration, through the use of a superpipeline that overlaps communication and memory copies. We have modeled the behavior of the network and proposed auto-tuning mechanism to adapt the protocol to the hardware properties.
6.4. Improve code-coupling performance in the SALOME platform

**Participants:** Alexandre Denis, Sébastien Barascou.

- SALOME platform is an open source software developed by EDF, CEA, and OpenCascade. It is an open simulation platform with pre-processing, post-processing, interoperability with CAD models, integration with computation kernels.
- YACS is the workflow engine used for code coupling applications in SALOME. It leverages CORBA for communications between kernels. We have ported YACS atop PadicoTM, our communication platform for grids. It enables CORBA connections to use InfiniBand networks. Benchmarks show a significant improvement in code coupling performance.

6.5. Hardware topology-aware MPI applications

**Participants:** Emmanuel Jeannot, Guillaume Mercier, François Tessier.

- We have expanded our previous work dealing with MPI process placement. Indeed, our approach relied on tools and techniques which were outside the scope of the MPI standard itself. In order to allow the users to utilize our work in a portable way, we enhanced some routines of the MPI standard. We worked mainly with the MPICH2 implementation but we are also working on an Open MPI version as well.
- Instead of modifying the binding of the MPI processes onto the physical cores on the underlying architecture, we chose to create a new communicator for which the logical topology organization is optimized for the hardware. This work has been published in [37] and show interesting performance improvements for some class of MPI applications.
- The problem of process placement, which can be reduced to a NP-hard graph partitioning problem, can be dealt with several famous applications like Scotch or ParMETIS. To evaluate these solutions with TREEMATCH, we ran several benchmarks using NAS Parallel Benchmarks and a real CFD application. On the one hand we study the quality of processes permutation (which will impact the execution time) and on the other hand the computation time of the permutation. These results will allow us to conclude about the pertinence of what graph partitioner can be used to bind processes on process units or to do a dynamic processes reordering.

6.6. Mastering Heterogeneous Platforms

**Participants:** Cédric Augonnet, Olivier Aumage, Ludovic Courtès, Nathalie Furmento, Andra Hugo, Raymond Namyst, Samuel Thibault, Pierre-André Wacrenier.

- We continued our work on extending STARPU to master exploitation of Heterogeneous Platforms.
- We have extended the STARPU scheduler into managing parallel tasks which permit a better exploitation of CPUs and load balancing with GPUs.
- We have designed over STARPU a lightweight DSM over MPI, which permits to seamlessly execute STARPU applications over an MPI cluster of GPU-enhanced nodes.
- We have been developing a GCC plug-in which extends the C language with pragmas and attributes that make writing STARPU applications a lot easier.
- We have brought to STARPU support for automatically converting data between CPU and GPU formats (typically arrays of structures vs structures of arrays). We are now optimizing it.
- We have added an OpenCL interface to STARPU, SOCL [42], which permits to execute unmodified OpenCL applications over STARPU.
- We have introduced in STARPU theoretical bound support [27]: from a record of the set of tasks submitted by the application, STARPU uses linear programming to give the execution time of an ideal scheduling, which can then be compared with the actual results.
- We have continued collaboration with the University of Tennessee, Knoxville for STARPU support in the state-of-the-art dense linear algebra library, Magma, in particular LU [26] and QR [27] factorizations. We have also collaborated with the University of Mons [41] and Linköping [32].
- Cédric Augonnet defended his PhD on STARPU [17].
6.7. Development of a flexible heterogeneous system-on-chip platform using a mix of programmable processing elements and hardware accelerators

Participants: Paul-Antoine Arras, Emmanuel Jeannot, Samuel Thibault.

- Today’s embedded applications are increasingly demanding in terms of computational power, especially in real-time digital signal processing (DSP) where tight timing requirements are to be fulfilled. More specifically, when it comes to video decoding (e.g. H.264/AVC) not only has it been almost impossible for some time to run such codecs on a stand-alone embedded processor, but it now also becomes quite impractical to execute them on homogeneous multicore platforms. In this context, STMicroelectronics is developing a scalable heterogeneous system-on-chip template called P2012 and aimed at meeting the latest codecs’ requirements.

- This year, the privileged axis of research was directed towards dataflow-based models, which benefit from such strong, well-known properties as analyzability, schedulability and expressivity. Furthermore, dataflow programming has already been used extensively in DSP, yielding a number of dedicated software synthesis tools. We have proposed a first version of the programming model that will be evaluated later.

6.8. Sparse GMRES on heterogeneous platforms in oil extraction simulation

Participants: Olivier Aumage, Corentin Rossignon, Samuel Thibault.

- We started a study on sparse matrix factorization and system resolution on heterogeneous platforms in collaboration with Pascal Hénon from company Total, in the context of oil extraction simulation. Sparse matrix computations are notoriously difficult to efficiently run on heterogeneous platforms in the general case due to the irregular memory access patterns they generate.

- However, in the specific context of this study, Corentin Rossignon showed as part of his Master Thesis [56] that the sparsity layout of matrices generated by such oil extraction simulation problems can lead to a much higher level of efficiency on heterogeneous platforms thanks when using a suitable sparse internal representation together with carefully written operators such as the sparse matrix-vector product together with the StarPU heterogeneous scheduler.

- Corentin Rossignon is now starting a Phd. Thesis in partnership with Total to build on these promising results.

6.9. Programming models for heterogeneous platforms

Participants: Olivier Aumage, Cyril Roelandt, Samuel Thibault, Ludovic Courtès.

- As part of Project FP3C with Japan, we started a study on to explore the use of StarPU as possible target runtime system for the XcalableMP language and compiler developed by Prof. Sato’s team from University of Tsukuba. XcalableMP is a pragma-based language designed for parallelising application on clusters of multicore processors. The compiler is responsible to expand XcalableMP pragma into complex work mapping, communication and data redistribution commands.

- The study of porting XcalableMP on top of StarPU was conducted by Cyril Roelandt during his Master Thesis [55], starting from the idea that computing node with one or more attached accelerating expansion cards can be seen as a distributed platform. The results of the study showed that on the one side, the power of the XcalableMP language itself is very interesting for the goal of simplifying the port of applications on heterogeneous platforms. However, a current assumption of the XcalableMP model is that the compiler does not insert implicit commands and behaviour except at the exact location of pragma annotations, which limit the range of optimizations available to the dynamic scheduler and memory manager of StarPU. We will thus continue to collaborate with Prof. Sato’s team within the FP3C to see how these limitations could be reduced or lifted when using XcalableMP with StarPU.
In an effort to make it easier for C programmers to benefit from StarPU, the team-project has been working on extensions to the C language allowing important StarPU concepts to be expressed concisely. These C extensions are provided as a plug-in for the GNU Compiler Collection (GCC), and is now distributed as part of StarPU. The GCC plug-in extends the syntax and semantics of C and related languages (C++, Objective-C) using attributes and pragmas. Attributes are used, for instance, to declare StarPU tasks and their implementations for the available targets (CPU, OpenCL, CUDA, etc.) Pragmas are used notably to provide programmers a way to describe data buffers that are passed to tasks, which in turn allows the StarPU run-time support to manage data transfers between main memory and GPUs as it sees fit. Finally, tasks are invoked like regular C functions.

In addition to easing application development, the GCC plug-in, thanks to its higher-level view of the program structure, is able to report certain classes of errors at compile-time, which would otherwise lead to run-time errors.

This project has been led by Ludovic Courtès of Inria’s Development and Experimentation Department (SED) at Bordeaux, as part of a joint development action with the SED.

6.10. Parallel Concha

Participants: Olivier Aumage, Marie-Christine Counilh.

- Within the ADT Ampli project, we contributed to the Concha CFD library developed by R. Becker’s Inria Team Concha in Pau. Together with R. Becker, E. Bergounioux and D. Trujillo from Concha Team, and François Rue from SED Bordeaux we designed and experimented with the MPI parallelization and the hybrid MPI+OpenMP parallelization of the library.
- The MPI parallelization is now finalized. The OpenMP level has been successfully tested on the Vanka smoother and is now being spread in the library. We will thus continue to contribute to this parallelization work, in particular with respect to the support of 3D simulation cases.

6.11. Scientific Application Analysis and Experiments

Participants: Olivier Aumage, Denis Barthou, Andres Charif-Rubial, François Tessier, Ludovic Stordeur.

- Within the context of the ANR ProHMPT project, we contributed a thorough analysis of hot spots, data structure usages and locality issues in memory accesses of an aerodynamics application from partner CEA CESTA.
- In accordance with these results, a new version of this application has been written by the CESTA Team with redesigned, locality-friendly data structures and simplified loop scheme. This new version performs much better than the previous one on both 2D and 3D cases.
- We also conducted tests about the port of selected kernels of this application on accelerated heterogeneous platforms. The results of these tests were disappointing with the first version of the application due to the layout of the main data structures that led to a lot of memory transfers between the central memory and the accelerated memory.
- We are now working on conducting these experiments with the redesigned version of the application whose new data structures should dramatically reduce the amount of data transfers.

1 See http://gcc.gnu.org/, for more information on GCC.
6.12. Virtualization of GPUs for OpenCL

Participants: Sylvain Henry, Alexandre Denis, Denis Barthou.

- We propose a new approach for OpenCL programming, using a unique virtual accelerator instead of using the physical accelerator. Placement on the real hardware is handled by the runtime instead of the user, improving productivity and performance scalability. This proposition relies on OpenCL standard but changes the way its API is used.
- We have shown on some simple examples how this approach, using StarPU as a runtime, enables executions with a better load balance and performance. We are working on how to generalize this to more complex benchmarks. This work has been presented in Renpar[ 42 ] workshop.

6.13. Automatically Adapting Task Grain for Hybrid Architectures

Participants: Sylvain Henry, Alexandre Denis, Denis Barthou.

- Given a parallel task graph, a runtime such as StarPU can place each task on different hardware. However, there is still the need to adapt the number of tasks, the granularity of these tasks, according to the target hardware. Due to architectures with CPUs and GPUs, it is potentially interesting to have tasks of different granularities. We explore transformations that enable to either automatically split tasks into small ones, or given some user knowledge on the tasks, decide how and when to split a large task into small ones.
- This work starts from a high-level representation of the code, using an explicit data-flow graph.

6.14. Performance modeling for power consumption reduction on the SCC

Participants: Bertrand Putigny, Brice Goglin, Denis Barthou.

- We build a model to predict performance of HPC code on the SCC ship. This model can predict runtime of regular code as well as power consumption for different frequency.
- This allows users to choose either to optimize power consumption, power efficiency or raw performance.
- This work has been published in an Intel Symposium [ 38 ].

6.15. Modeling cache coherence protocol overhead

Participants: Bertrand Putigny, Denis Barthou, Brice Goglin.

- We are building a fine grained cache model to understand common cache coherence issue.
- This model is built on a set of micro-benchmarks and can also be used to improve find some bottlenecks in memory bound code. Our set of micro-benchmarks can also be used as a test bed for new architectures [ 54 ].

6.16. Memory Performance Analysis and Tool for OpenMP codes

Participants: Andres Charif-Rubial, Denis Barthou.

- We propose a performance analysis of OpenMP codes, based on memory accesses and cache hierarchies.
- This analysis relies on memory traces for multi-threaded codes and on static analysis of binary code. Memory traces are obtained through MAQAO by static binary rewriting and are compressed online, building polyhedral iteration domains. The static analysis, mostly induction variable detection on binary code, provides the same analysis whenever possible, removing the need in some cases for dynamic instrumentation.
- The analysis focuses on a number of issues in multi-threaded executions: thread affinity issues, false sharing, cache pollution.
- This work is in collaboration with Exascale Computing Lab.
6.17. Data-layout Optimization for Stencil codes on multi-cores and GPUs

Participants: Julien Jaeger, Denis Barthou.

- We develop a new approach for stencil code generation, optimizing data-layout for multi-threaded, SIMD code on multicores and CUDA code on GPU. The transformation handles different stencil parameters, and memory constraints.
- The code generated reaches high levels of performance, outperforming related works for multicores and with similar performance on GPUs. This work is submitted to publication and was first presented in a workshop [52].