Activity Report 2012

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5. Software

5.1. AeroSol

Participants: Damien Genêt [corresponding member for Bacchus], Maxime Mogé, Dragan Amenga-Mbengoué, François Pellegrini, Vincent Perrier [corresponding member], Mario Ricchiutto, François Rue.

The Aerosol software is jointly developed by teams BACCHUS and Cagire. It is a high order finite element library written in C++. The design has been carried for being able to perform efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The distribution of the unknowns is made with the software PaMPA, developed within teams BACCHUS and PUMAS. Maxime Mogé has been hired on a young engineer position (IJD) obtained in the ADT 0uBa HOP for participating in the parallelization of the library, and arrived on November, 1st 2011. On January 2012, Dragan Amenga-Mbengoué was recruited on the ANR Realfluids.

At the end of 2011, Aerosol had the following features:

- Development environment: use of CMake for compilation,CTest for automatic testing and memory checking, lcov and gcov for code coverage reports.
- In/Out: link with the XML library for handling with parameter files. Reader for GMSH, and writer to the VTK-ASCII legacy format.
- Quadrature formula: up to 11th order for Lines, Quadrangles, Hexaedra, Pyramids, Prisms, up to 14th order for tetrahedron, up to 21st order for triangles.
- Finite elements: up to fourth degree for Lagrange finite elements on lines, triangles and quadrangles.
- Geometry: elementary geometrical functions for first order lines, triangles, quadrangles.
- Time iteration: explicit Runge-Kutta up to fourth order, explicit Strong Stability Preserving schemes up to third order.
- Linear Solvers: link with the external linear solver UMFPack.
- Memory handling: discontinuous and continuous discretizations based on PaMPA for triangular and quadrangular meshes.
- Numerical schemes: continuous Galerkin method for the Laplace problem (up to fifth order) with non consistent time iteration or with direct matrix inversion. Scalar stabilized residual distribution schemes with explicit Euler time iteration have been implemented for steady problems.

This year, the following features were added:

- Development environment: development of a CDash server for collecting the unitary tests and memory checking. Beginning of the development of an interface for functional tests.
- General structure: Parts of the code were abstracted in order to allow for parallel development: Linear solvers (template type abstraction for generic linear solver external library), Generic integrator classes (integrating on elements, on faces with handling neighbor elements, or for working on Lagrange points of a given element), models (template abstraction for generic hyperbolic systems), equations of state (template-based abstraction for a generic equation of state).
- In/Out: Parallel GMSH reader, cell and point centered visualization based on VTK-legacy formats. XML paraview files on unstructured meshes (vtu), and parallel XML based files (pvtu).
- Quadrature formula: Gauss-Lobatto type quadrature formula.
- Finite elements: Hierarchichal orthogonal finite element basis on lines, triangles (with Dubiner transform). Finite element basis that are interpolation basis on Gauss-Legendre points for lines, quadrangles, and hexaedra. Lagrange, and Hierarchical orthogonal finite elements basis for hexaedra, prisms and tetrahedra.
• Geometry: elementary geometrical functions for first order three dimensional shapes: hexaedra, prisms, and tetrahedra.
• Time iteration: CFL time stepping, optimized CFL time schemes: SSP(2,3) and SSP (3,4)
• Linear Solvers: Internal solver for diagonal matrices. Link with the external solvers PETSc and MUMPS.
• Memory handling: parallel degrees of freedom handling for continuous and discontinuous approximations
• Numerical schemes: Discontinuous Galerkin methods for hyperbolic systems. SUPG and Residual Distribution schemes.
• Models: Perfect gas Euler system, real gas Euler system, scalar advection, Waves equation in first order formulation, generic interface for defining space-time models from space models.
• Numerical fluxes: centered fluxes, exact Godunov’ flux for linear hyperbolic systems, and Lax-Friedrich flux.
• Parallel computing: Mesh redistribution, computation of Overlap with PaMPA. Collective asynchronous communications (PaMPA based). Tests on the cluster Avakas from MCIA, and on Mésocentre de Marseille. The library was also compiled on PlaFRIM.
• C++/Fortran interface: Tests for binding fortran with C++.

5.2. COCA
Participants: Mario Ricchiuto [corresponding member], Gérard Vignoles.

COCA (CodeOxydationCompositesAutocicatrisants) is a Fortran 90 code for the simulation of the oxidation process in self-healing composite materials, developed in collaboration with the Laboratoire des Composites ThermoStructuraux in Bordeaux (UMR-5801 LCTS). This process involves the chemical oxidation of some of the matrix components of the composite, and the production of a liquid oxide that flows and fills material cracks, acting as a diffusion barrier against oxygen and thus protecting the ceramic fibers of the material. COCA simulates this process using a finite element discretization of the model equations. In its current version only transverse cracks are available. COCA makes use of PaStiX to solve the algebraic systems arising from the discretization.

5.3. RealfluiDS
Participants: Dante de Santis, Gianluca Geraci, Pietro Marco Congedo, Rémi Abgrall [corresponding member].

RealfluiDS is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multimaterial, MHD flows and turbulent flows (using the SA model). There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in the 3D one. This software implements the more recent residual distribution schemes. The code has been parallelized with and without overlap of the domains. An Uncertainty Quantification library has been added to the software. A partitioning tool exists in the package, which uses Scotch. In the years to come, all the know-how of RealfluiDS will be transferred to Aerosol.

5.4. MMG3D
Participants: Cécile Dobrzynski [corresponding member], Algiane Froehly.
MMG3D is a tetrahedral fully automatic remesher. Starting from a tetrahedral mesh, it produces quasi-uniform meshes with respect to a metric tensor field. This tensor prescribes a length and a direction for the edges, so that the resulting meshes will be anisotropic. The software is based on local mesh modifications and an anisotropic version of Delaunay kernel is implemented to insert vertices in the mesh. Moreover, MMG3D allows one to deal with rigid body motion and moving meshes. When a displacement is prescribed on a part of the boundary, a final mesh is generated such that the surface points will be moved according this displacement. MMG3D is used in particular in GAMMA for their mesh adaptation developments, but also at EPFL (maths department), Dassault Aviation, Lemma (a french SME), etc. MMG3D can be used in FreeFem++ (http://www.freefem.org), a free software which eases the solving of PDEs and in Gmsh (http://geuz.org/gmsh/). More details can be found on http://www.math.u-bordeaux1.fr/~dobj/logiciels/mmg3d.php.

A new version of MMG3D is under development. The big novelty of this version is the modification of the surface triangulation. A. Froehly, ingenieer in the FUI Rodin, is working on this new version.

5.5. ORComp
Participants: Pietro Marco Congedo [Corresponding member], Rémi Abgrall, Nassim Razaaly, Dante De Santis, Maria-Giovanna Rodio.

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

5.6. PaMPA
Participants: Cédric Lachat, François Pellegrini [Corresponding member], Cécile Dobrzynski, Hervé Guillard [PUMAS], Laurent Hascoët [Tropics].

PaMPA ("Parallel Mesh Partitioning and Adaptation") is a middleware library dedicated to the management of distributed meshes. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution. It is based on a distributed data structure that represents meshes as a set of entities (elements, faces, edges, nodes, etc.), linked by relations (that is, computation dependencies).

PaMPA interfaces with Scotch for mesh redistribution, and with MMG3D for parallel remeshing of tetrahedral elements. Other sequential remeshers can be plugged in order to handle other types of elements.

Version 0.2 allows users to declare a distributed mesh, to declare values attached to the entities of the meshes (e.g. temperature attached to elements, pressures to the faces, etc.), to exchange values between overlapping entities located at the boundaries of subdomains assigned to different processors, to iterate over the relations of entities (e.g. iterate over the faces of elements), to remesh the pieces of the mesh that need to, and to redistribute evenly the remeshed mesh across the processors of the parallel architecture.

PaMPA is already used as the data structure manager for two solvers being developed at Inria: Plato and Aerosol.

5.7. PLATO
Participants: Hervé Guillard [PUMAS], Laure Combe [PUMAS,contact], Cédric Lachat, Pierre Ramet [corresponding member].
The development of Plato ("A platform for Tokamak simulation") (http://www-sop.inria.fr/pumas/plato.php) is being supported by an ADT action of the D2T. Plato is a suite of data and software dedicated to the geometry and physics of Tokamaks and its main objective is to provide the Inria large scale initiative FUSION teams working with plasma fluid models with a common development tool. The construction of this platform will integrate the following developments.

1. A (small) database corresponding to axi-symmetrical solutions of the equilibrium plasma equations for realistic geometrical and magnetic configurations (ToreSupra, JET and ITER). The construction of meshes is always an important time consuming task. Plato will provide meshes and solutions corresponding to equilibrium solutions that will be used as initial data for more complex computations.

2. A set of tools for the handling, manipulation and transformation of meshes and solutions using different discretisations (P1, Q1, P3, etc)

3. Numerical templates allowing the use of 3D discretization schemes using finite element schemes in the poloidal plane and spectral Fourier or structured finite volume representations in the toroidal one.

4. Several applications (Ideal MHD and drift approximation) used in the framework of the Inria large scale initiative FUSION.

5.8. RobUQ

Participants: Pietro Marco Congedo [Corresponding member], Rémi Abgrall, Gianluca Geraci, Julie Tryoen, Nassim Razaaly.

The RobUQ platform has been conceived to solve problems in uncertainty quantification and robust design. It includes the optimization code ALGEN, and the uncertainty quantification code NISP. It includes also some methods for the computation of high-order statistics, efficient strategies for robust optimization, the Simplex2 method. Some methods are developed in partnership with the Stanford University (in the framework of the associated team AQUARIUS). Other methods are developed in the context of ANR UFO.

5.9. Scotch

Participants: François Pellegrini [corresponding member], Sébastien Fourestier.

parallel graph partitioning, parallel static mapping, parallel sparse matrix block ordering, graph repartitioning, mesh partitioning.

Scotch (http://www.labri.fr/~pelegrin/scotch/) is a software package for parallel and sequential sparse matrix ordering, parallel and sequential graph partitioning, as well as sequential static mapping and remapping, without and with fixed vertices, and mesh and hypergraph partitioning.

The initial purpose of Scotch was to compute high-quality static mappings of valued graphs representing parallel computations onto target architectures of arbitrary topologies. This allows the mapper to take into account the topology and heterogeneity of the target architecture in terms of processor speed and link bandwidth. This feature, which was meant for the NUMA machines of the 1980’s, has not been widely used in the past because machines in the 1990’s became UMA again thanks to hardware advances. Now, architectures become NUMA again, and these features are regaining popularity.

Version 5.0 of Scotch, released on August 2007, was the first version to comprise parallel routines. This extension, called PT-Scotch (for “Parallel Threaded Scotch”), is based on a distributed memory model, and makes use of the MPI and, optionally, Posix thread APIs. Version 5.1, released on September 2008, extended the parallel features of PT-Scotch, which can now compute graph partitions in parallel by means of a parallel recursive bipartitioning framework. Release 5.1.10 had made Scotch the first full 64-bit implementation of a general purpose graph partitioner.
Version 6.0, released on December 2012, corresponding to the 20-year anniversary of Scotch, offers many new features: static mapping with fixed vertices, static remapping, and static remapping with fixed vertices. Several critical algorithms of the formerly sequential Scotch library can now run in a multi-threaded way. All of these features will be available for the parallel PT-Scotch library in the upcoming release 6.1.

Scotch has been integrated in numerous third-party software, which indirectly contribute to its diffusion, e.g. OpenFOAM (fluid mechanics solver, OpenCFD Ltd.), the CODE_ASTER LIBRE solver (thermal and mechanical analysis software developed by French state-owned electricity producer EDF), the ZOLTAN module of the TRILINOS software (SANDIA Labs), the parallel linear system solvers MUMPS (ENSEEIT/IRIT, LIP and LaBRI), SuperLUDist (U.C. Berkeley), PaStiX (LaBRI) and HIPS (LaBRI), etc. Scotch is natively available in several Linux and Unix distributions, as well as on some vendors platform (SGI, etc).

5.10. SLOWS

Participant: Mario Ricchiuto [corresponding member].

SLOWS (“Shallow-water FLOWS”) is a C-platform allowing the simulation of free surface shallow water flows with friction. Arbitrary bathymetries are allowed, defined either by some complex piecewise analytical expression, or by xyz data files, the classical Manning model for friction is used, and an Exner model is implemented for sediment transport. The equations are discretized with a residual based approach which is an adaptation of the schemes developed for aeronautics applications. Due to the inherent unsteadiness of these flows, the time discretization plays an important role. Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach.
5. Software

5.1. Softwares


We have developed various prototype software but, currently, they are not distributed and used only within the project. Regarding software, we know (see the last LIAMA evaluation report) that we should consider disseminating some of its codes more widely. Using established libraries may improve the impact of some of the results. We did not do it, due to the fast turn over of students in the Chinese team and the lack of Manpower and know-how in the French part.
CAGIRE Team

5. Software

5.1. AeroSol

Participants: Dragan Amenga-Mbengoué [Bacchus], Damien Genet [Bacchus], Maxime Mogé, François Pellegrini [Bacchus], Vincent Perrier [correspondant], François Rué [Bacchus], Mario Ricchiuto [Bacchus].

The software AeroSol is jointly developed in the team Bacchus and the team Cagire. It is a high order finite element library written in C++. The code design has been carried for being able to perform efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The distribution of the unknowns is made with the software PaMPA, developed within the team Bacchus and the team Pumas. This year, Dragan Amenga-Mbengoué was recruited on the ANR Realfluids, and François Rué (Service Experimentation et Développement) joined the team Bacchus for working on Aerosol.

At the end of 2011, Aerosol had the following features

- **development environement** use of CMake for compilation, CTest for automatic tests and memory checking, lcov and gcov for code coverage reports.
- **In/Out** link with the XML library for handling with parameter files. Reader for GMSH, and writer on the VTK-ASCII legacy format.
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- **Models** Perfect gas Euler system, real gas Euler system, scalar advection, Waves equation in first order formulation, generic interface for defining space-time models from space models.

- **Numerical fluxes** centered fluxes, exact Godunov’ flux for linear hyperbolic systems, and Lax-Friedrich flux.

- **Parallel computing** Mesh redistribution, computation of Overlap with PaMPA. collective asynchronous communications (PaMPA based). Tests on the cluster Avakas from MCIA, and on Mésocentre de Marseille, and PlaFRIM.

- **C++/Fortran interface** Tests for binding fortran with C++.
5. Software

5.1. SeLaLib

**Participants:** Raphaël Blanchard, Edwin Chacon Golcher, Samuel De Santis, Aliou Diouf, Pierre Navaro, Morgane Bergot, Emmanuel Frénod, Philippe Helluy, Sever Hirstoaga, Michel Mehrenberger, Laurent Navoret, Eric Sonnendrücker.

Under the 'Fusion' large scale initiative, we have continued our work in the development of the ADT Selalib (the Semi-Lagrangian Library), now finishing its second year. This library provides building blocks for the development of numerical simulations for the solution of the fundamental equation of plasma physics: the Vlasov equation. In this context we have continued to add new modules improved interfaces and implemented 'continuous integration’ software development techniques to improve code robustness and portability. Furthermore, we continue to involve other researchers within France and abroad to aid in the further development of this software product.

One of the aims of the ADT is to provide numerical building blocks for the GYSELA code developed at CEA Cadarache in collaboration with the Calvi project-team. GYSELA is used by physicists for simulating the development of turbulence in magnetic fusion plasmas in particular in view of the ITER project.

5.2. CLAC

**Participants:** Anaïs Crestetto, Philippe Helluy.

The objective of the three-dimensional parallel software CM2 (Code Multiéchelle Multiphysique) software is to implement a general solver for hyperbolic conservation laws. It is for instance able to solve the MHD model. CLAC is a C++ OpenCL/MPI based library derived from algorithms and ideas developed in CM2. CLAC means “Compute Language Approximation of Conservation laws”.

It is clear now that a future supercomputer will be made of a collection of thousands of interconnected multicore processors. Globally it appears as a classical distributed memory MIMD machine. But at a lower level, each of the multicore processors is itself made of a shared memory MIMD unit (a few classical CPU cores) and a SIMD unit (a GPU). When designing new algorithms, it is important to adapt them for this architecture. Our philosophy will be to program our algorithms in such a way that they can be run efficiently on this kind of computers. Practically, we will use the MPI library for managing the high level parallelism, while the OpenCL library will efficiently operate the low level parallelism.

We have invested for several years now into scientific computing on GPU, using the open standard OpenCL (Open Computing Language). With Anaïs Crestetto, who is preparing a PhD in the CALVI project, we were recently awarded a prize in the international AMD OpenCL innovation challenge thanks. We have developed an OpenCL 2D Vlasov-Maxwell solver, coupling a PIC and a DG algorithms, which fully runs on a GPU. OpenCL is a very interesting tool because it is an open standard now available on almost all brands of multicore processors and GPU. The same parallel program can run on a GPU or a multicore processor without modification.

CLAC is written in C++, which is almost mandatory, because we use the OpenCL library. It also uses the MPI paradigm and is thus able to run on a cluster of GPU. CLAC is also inside a collaboration with a Strasbourg SME, AxesSim, which develops software for electromagnetic simulations. Thomas Strub, who is employed in AxesSim with a CIFRE position, is doing his Ph. D. on the conception and the development of CLAC applied to electromagnetic problems.

Because of the envisaged applications of CLAC, which may be either academical or commercial, it is necessary to conceive a modular framework. The heart of the library is made of generic parallel algorithms for solving conservation laws. The parallelism can be both fine grain (oriented towards GPU and multicore processors) and large grain (oriented towards GPU clusters). The separated modules allow managing the meshes and some specific applications. In this way, it is possible to isolate parts that can be protected by trade secret.
CASTOR Team

4. Software

4.1. FluidBox

Participants: Boniface Nkonga [contact], Hervé Guillard.

FluidBox is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multi-material and MDH flows. There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in 3D. Two classes of schemes are available: A classical finite volume scheme and the more recent residual distribution schemes. Several low Mach number preconditioning are also implemented. The code has been parallelized with and without domain overlapping. The linear solver PaStiX is integrated in FluidBox. A partitioning tool exists in the package and uses Scotch. At present the software is only a private project but some parts of FluidBox are expected to be in the public domain by the end of the year.

4.2. PlaTo

Participants: Hervé Guillard [contact], Laure Combe.

The development of PlaTo (A platform for Tokamak simulation) (http://www-sop.inria.fr/pumas/plato.php) has been supported by an ADT action of the D2T and by the ANR ESPOIR. PlaTo is a suite of data and softwares dedicated to the geometry and physics of Tokamaks and its main objective is to provide the Inria large scale initiative “FUSION” teams working in plasma fluid models with a common development tool.

4.3. PaMPA

Participants: Cécile Dobrzynski [Bacchus], Hervé Guillard, Laurent Hascoët [Tropics], Cédric Lachat, François Pellegrini [Bacchus].

PaMPA (“Parallel Mesh Partitioning and Adaptation”) is a middleware library dedicated to the management of distributed meshes. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution. An API of the future platform has been devised, and the coding of the mesh handling and redistribution routines is in progress. PaMPA will be used as a base module for the PLATO solvers, to balance dynamically, refine and coarsen its distributed mesh.

4.4. Cedres++

In Tokamaks, at the slow resistive diffusion time scale, the magnetic configuration in the plasma can be described by the MHD equilibrium equations inside the plasma and the Maxwell equations outside. Moreover, the magnetic field is often supposed not to depend on the azimuthal angle.

Under this assumption of axisymmetric configuration, the equilibrium in the whole space reduces to solving a 2D problem in which the magnetic field in the plasma is described by the well known Grad Shafranov equation. The unknown of this problem is the poloidal magnetic flux. The P1 finite element code CEDRES++ solves this free boundary equilibrium problem in direct and inverse mode. The direct problem consists in the computation of the magnetic configuration and of the plasma boundary, given a plasma current density profile and the total current in each poloidal field coils (PF coils). The aim of the inverse problem is to find currents in the PF coils in order to best fit a given plasma shape. An evolutive version of the code has also been recently developed. This version takes into account the circuit equations in the PF coils. These equations give a time dependent relation between the voltages, the total current in the coils and the time derivative of the magnetic flux. Induced currents in passive structures like the vacuum vessel are also considered in this dynamic equilibrium problem. This new version of the code is an important tool for plasma scenario development and Tokamak design studies.
4.5. Equinox

EQUINOX is a code dedicated to the numerical reconstruction of the equilibrium of the plasma in a Tokamak. The problem solved consists in the identification of the plasma current density, a non-linear source in the 2D Grad-Shafranov equation which governs the axisymmetric equilibrium of a plasma in a Tokamak. The experimental measurements that enable this identification are the magnetics on the vacuum vessel, but also polarimetric and interferometric measures on several chords, as well as motional Stark effect measurements. The reconstruction can be obtained in real-time and the numerical method implemented involves a finite element method, a fixed-point algorithm and a least-square optimization procedure.
COFFEE Project-Team

5. Software

5.1. NS2DDV

The code NS2DDV is developed jointly with the team SIMPAF, of the Inria Research Centre Lille Nord Europe. It is devoted to the simulation of non-homogeneous viscous flows, in two-dimensional geometries. The code is based on an original hybrid Finite Volume/Finite Element scheme; it works on unstructured meshes and can include mesh refinements strategies. Further details can be found in the research papers J. Comput. Phys., 227, 4671–4696, 2008 and J. Comput. Phys., 229 (17), 6027–6046, 2010. The code exists in two versions: a Matlab public version, a C++ prototype version allowing more ambitious simulations. Both versions are still subject to developments. The current versions is restricted to incompressible flows but on-going progress are concerned with the simulation of avalanches. The source code of the public version is downloadable and several benchmarks tests can be reproduced directly.

5.2. FV_PM

We are developing codes based on Finite Volume discretization, for the (2d and 3d) simulations of multiphase flows in porous media. For instance these methods apply to the simulation of problems motivated by CO2 storage, oil recovery or nuclear waste depository. A preliminary version, the code ComPASS (Computing Parallel Architecture to Speed up Simulations), which includes parallel procedures, has been recently developed, through a successful CEMRACS project.

5.3. SimBiof

We are developing numerical methods, currently by using Finite Differences approaches, for the simulation of biofilms growth. The underlying system of PDEs takes the form of multiphase flows equations with conservation constraints and vanishing phases. The numerical experiments have permitted to bring out the influence of physical parameters on the multidimensional growth dynamics.

5.4. AP_PartFlow

We are developing experimental codes, mainly based on Finite Differences, for the simulation of particulate flows. A particular attention is paid to guaranty the asymptotic properties of the scheme, with respect to relaxation parameters.
5. Software

5.1. C++ library Concha

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

The objectives of our library CONCHA are to offer a flexible and extensible software with respect to:
- Numerical methods and
- Physical models.

The aim is to have a flexible code which could easily switch between the different discretizations, in order to provide a toolbox for rapid testing of new ideas.

The software architecture is designed in such a way that a group of core developers can contribute in an efficient manner, and that independent development of different physical applications is possible. Further, in order to accelerate the integration of new members and in order to provide a basis for our educational purposes (see Section 8.1), the software proposes different entrance levels. The basic structure consists of a common block, and several special libraries which correspond to the different fields of applications described in Sections 4.1 – 4.4. Hyperbolic solvers, Low-Mach number flow solvers, DNS, and viscoelastic flows. A more detailed description of each special library may be found below. In order to coordinate the cooperative development of the library, Concha is based on the Inria-Gforge.

5.2. User interface and python interface

Participants: Roland Becker, David Trujillo.

![Graphical user interface: option panel (left) and process panel (right) of the install tool.](image)

We are confronted with heterogenous backgrounds and levels of implication of the developers and users. It seems therefore crucial to be able to respond to the different needs. Our aim is to facilitate the development of the library, and at the same time, to make it possible that our colleagues involved in physical modeling can have access to the functionality of the software with a reasonable investment of time. Two graphical user interfaces have been developed: one for the installation of the library and another one for the building and execution of projects. They are based on common database and scripts written in python. The scripts can also be launched in a shell. In Figure 3 the user interface of the install tool is shown. The option panel allows to choose the components for conditional compilation and the compilation type (debug and release).
In Figure 4 the user interface of the project tool is shown. A project consists of a number of sources files and a parameter file used by the C++-executable. The sources define classes derived from the library, which are used to specify certain data such as boundary conditions and employed finite element spaces. The parameter file contains algorithmic information and physical parameters. It is generated from a database by the python utilities.

The tools offered by this development platform are based on a python interface for the library, called pyConcha. It offers a common interface, based on a pluggin-system, which allows the devoIopment of command line tools in parallel. This year the consolidation of the interface part of pyConcha has been an important task. The pyConcha library is now a framework rather than a simple interface to Concha C++ library. It allows now creation of plugins, so that each user-programmer can customize pyConcha to his own goals. Previously, two main programs were working: concha-install.py to install library, and concha-project.py for (semi-)end-users. Both are now plugins of pyConcha, and can be launched by pyConcha at startup. A plugin visualization could now be developed in an independant way, and launched by pyConcha on demand.

The structure of pyConcha framework is clearly splitted in various modules(layers): Command Line Interface module, Graphical User Interface module and Handlers modules, see Figure 5 . A great effort has been made for internationalization of pyConcha.

5.3. Euler equations

Participants: Roland Becker, Kossivi Gokpi, Robert Luce, Eric Schall, David Trujillo.

Based on the library CONCHA we have developed a solver for hyperbolic PDE’s based on DGFM. So far different standard solvers for the Euler equations such as Lax-Friedrichs, Steger-Warming, and HLL have been implemented for test problems. A typical example is the scram jet test case shown in Figure 6.

5.4. Incompressible flow solvers

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

We have started the validation of the implementation of different finite element methods for incompressible flows at hand of standard benchmark problems as the Stokes flow around a symmetric cylinder [65] and the stationary flow around a slightly non symmetric cylinder [70], see Figure 7.
Figure 5. Structure of the pyConcha framework.

Figure 6. Computed Mach-number distribution for the Scramjet test problem.
5.5. DNS

Participants: Roland Becker, David Trujillo.

For the direct numerical simulation of incompressible turbulent flows, we have started to develop a special solver based on structured meshes with a fast multigrid algorithm incorporating projection-like schemes. The main idea is to use non-conforming finite elements for the velocities with piecewise constant pressures, leading to a special structure of the discrete Schur complement, when an explicit treatment of the convection and diffusion term is used.

5.6. Validation and comparison with other CFD-software

Participants: Roland Becker, Didier Graebling, Eric Schall, David Trujillo.

Validation and comparison with other CFD-software is crucial in order to evaluate the potential of our numerical schemes concerning accuracy, computing time and other practical aspects.

We have compared the Concha library for incompressible and compressible flows. For incompressible flows, we have used a test case proposed by Hulsen and the well-known Schafer-Turek cylinder benchmark in order to validate the accuracy of the Stokes and Navier-Stokes solvers. The viscoelastic code has been compared with PolyFlow for different test configurations.

The compressible Euler code has been compared to the ELSA software developed by ONERA.

For further comparison and validation, it would be important to consider other commercial and research tools such as: Aéro3 (Inria-Smash), AVBP (CERFACS), Fluent (ANSYS), and OpenFOAM (OpenCfd).

For this purpose we have proposed the ADT-project VALUE in collaboration with a small company involved in aerodynamics (EPSILON Toulouse), which unfortunately has been rejected by Inria.
5. Software

5.1. RODIN

Participant: Grégoire Allaire [correspondant].

RODIN project: developing an industrial software for geometry and topology optimization of solid structures, based on the level set method.

5.2. FreeFem++ Toolboxes

5.2.1. Shape optimization toolbox in FreeFem++

Participants: Grégoire Allaire, Olivier Pantz.

We propose several FreeFem++ routines which allow the users to optimize the thickness, the geometry or the topology of elastic structures. All examples are programmed in two space dimensions. These routines have been written by G. Allaire, B. Boutin, C. Dousset, O. Pantz. A web page of this toolbox is available at http://www.cmap.polytechnique.fr/~allaire/freefem_en.html.

We also have written a C++ code to solve the Hamilton-Jacobi equation used in the Level-set shape optimization method. This code has been linked with FreeFem++ routines.

5.2.2. Inverse shape and medium problem for thin coatings

Participant: Nicolas Chaulet.

We developed a FreeFem++ toolbox which retrieve an obstacle and two coefficients that define a generalized impedance boundary condition form a few far field data in dimension 2. The reconstruction algorithm relies on regularized non linear optimization technique. The toolbox also contains a forward solver for the scattering of acoustic waves by obstacle on which a generalized impedance boundary condition is applied using an approximate Dirichlet-to-Neuman map to bound the computational domain.

5.2.3. Inverse shape problems for axisymmetric eddy current problems

Participant: Zixian Jiang.

This FreeFem++ toolbox solves inverse problems for an axisymmetric eddy current model using shape optimization techniques. The underlying problem is to find inclusions in a tubular and unbounded domain. The direct scattering problems are solved using an adaptive finite element method, and Dirichlet-to-Neumann operators are used to implement the transparent boundary conditions. Based on the shape derivative of an inclusion with respect to the domain, the toolbox offers regularized iterative algorithms to solve the inverse problem.

5.2.4. Contact managements

Participant: Olivier Pantz.

We have developed a toolbox running under FreeFem++ in order to take into account the non-intersection constraints between several deformable bodies. This code has been used to treat contacts between red blood cells in our simulations, but also between genuine non linear elastic structure. It can handle both contacts and self-contacts.

Moreover, a toolbox based on the Penalization method has also been developed.

5.2.5. De-Homogenization

Participant: Olivier Pantz.
We have developed a code under Freefem++ that implements our De-Homogenization method. It has been used to solve the compliance minimization problem of the compliance of an elastic shape. In particular, it enables us to recover well known optimal Michell’s trusses for shapes of low density.

5.3. Scilab and Matlab Toolboxes

5.3.1. Shape optimization toolbox in Scilab
Participant: Grégoire Allaire [correspondant].

Together with Georgios Michailidis, we improved a Scilab toolbox for 2-d shape and topology optimization by the level set method which was originally produced by Anton Karrman and myself. The routines, a short user’s manual and several examples are available on the web page: http://www.cmap.polytechnique.fr/~allaire/levelset_en.html

5.3.2. Conformal mapping method
Participant: Houssem Haddar [correspondant].

This Scilab toolbox is dedicated to the resolution of inverse 2-D electrostatic problems using the conformal mapping method introduced by Akdumann, Kress and Haddar. The toolbox treats the cases of a simply connected obstacle with Dirichlet, Neumann or impedance boundary conditions or a simply connected inclusion with a constant conductivity. The latest development includes the extension of the method to the inverse scattering problem at low frequencies as introduced by Haddar-Kress (2012).

5.3.3. Direct and inverse problems in waveguides
Participants: Armin Lechleiter [correspondant], Dinh Liem Nguyen.

This Matlab toolbox includes fast solvers for direct and inverse scattering problems in planar 3D waveguides for inhomogeneous media. The direct scattering problems are solved using an spectral integral equation approach relying on the Lippmann-Schwinger integral equation, discretized as a Galerkin method via the fast Fourier transform. The toolbox includes preconditioning by a two-grid scheme and multipole expansions coupled to the spectral solver to allow for multiple scattering objects. The inverse problem to find the shape of the scattering object from near-field measurements is solved using a Factorization method.

5.4. Sampling methods for inverse problems

5.4.1. Samplings-2d
Participant: Houssem Haddar [correspondant].

This software is written in Fortran 90 and is related to forward and inverse problems for the Helmholtz equation in 2-D. It includes three independent components. The first one solves to scattering problem using integral equation approach and supports piecewise-constant dielectrics and obstacles with impedance boundary conditions. The second one contains various samplings methods to solve the inverse scattering problem (LSM, RGLSM(s), Factorization, MuSiC) for near-field or far-field setting. The third component is a set of post processing functionalities to visualize the results. See also the web page http://sourceforge.net/projects/samplings-2d/.
- License: GPL
- Type of human computer interaction: sourceforge
- OS/Middleware: Linux
- Programming language: Fortran
- Documentation: fichier

5.4.2. Samplings-3d
Participant: Houssem Haddar [correspondant].
This software is written in Fortran 90 and is related to forward and inverse problems for the Helmholtz equation in 3-D. It contains equivalent functionalities to samplings-2d in a 3-D setting.

5.4.3. Time domain samplings-2d

Participants: Houssem Haddar [correspondant], Armin Lechleiter.

This software is written in Fortran 90 and is related to forward and inverse problems for the time dependent wave equation in 2-D. The forward solver is based on a FDTD method with PMLs. The inverse part is an implementation of the linear sampling method in a near field setting and the factorization method in a far field setting.

5.4.4. Factorization Method for EIT

Participants: Giovanni Migliorati.

We developed a numerical code that implements the Factorization Method applied to the Continuous Model, in the framework of Electrical Impedance Tomography featuring an inhomogeneous background. The numerical scheme relies on the approximation by the finite element method of the solution to the dipole-like Neumann boundary-value problem. Two regularization techniques are implemented, i.e. the Tikhonov regularization embedding Morozov principle, and the classical Picard Criterion. The code now supports the case of piecewise-wise constant by unknown background.

5.5. BlochTorreyPDESolver

Participants: Jing-Rebecca Li [correspondant], Dang Van Nguyen.

We developed numerical codes to solve the multiple compartment Bloch Torrey partial differential equation in 2D and 3D to simulate the bulk magnetization of a sample under the influence of a diffusion-encoding gradient magnetic field. We coupled a mass-conserving spatial discretization with a stable time discretization using an explicit Runge-Kutta-Chebyshev method and we are able to solve the Bloch-Torrey PDE in multiple compartments for an arbitrary diffusion sequence with reasonable accuracy for moderately complicated geometries in computational time that is on the order of tens of minutes per bvalue on a laptop computer.

This code has been implemented in Fortran90, C++, as well as Matlab. A Matlab Toolbox with graphical user interface for the simulation of DMRI signals in 2D and 3D cellular geometries using this numerical method is being developed.

The version of the code using Finite Volume discretization on a Cartesian grid is complete (written by Jing-Rebecca Li). The version of the code using linear Finite Elements discretization is in the final testing phase (written by Dang Van Nguyen).

See the web page http://www.cmap.polytechnique.fr/~jingrebeccali/ for more details.
GAMMA3 Project-Team (section vide)
IPSO Project-Team (section vide)
MC2 Project-Team

5. Software

5.1. eLYSe

Participants: Olivier Saut [correspondant], Raphael Bahègne, Vincent Huber, Jean-Baptiste Lagaert, Mathieu Specklin.

eLYse is a numerical platform used for our computations in Biology (tumor growth), micro-fluidics and complex Newtonian fluid flows. The platform is divided in two libraries: one is devoted to the modelling equations and the other one includes the numerical solvers. For example, we are able to treat (in 2D and 3D) transport equations, diffusion equations, Navier-Stokes equations, Maxwell system and the interaction fluid-structure by level-set and penalization methods. The solvers are based on finite volume methods on cartesian grids and allow parallel computations. See also the web page http://www.math.u-bordeaux1.fr/~osaut/pages/eLYSe.html.

- Version: 0.4
- ACM: ACM J.2 J.3 G.1.8 G.1.10
- AMS: AMS65Z05 35Q92
- Keywords: Modélization and numerical simulations, Finite volume methods, Level Set approach, Penalization method
- APP: En cours
- Type of human computer interaction: console
- OS/Middelware: Platform developped on Mac OS X architecture.
- Programming language: C++
- Documentation: doxygen.

5.2. Kesaco

Participants: Olivier Saut [correspondant], Raphael Bahègne, Damiano Lombardi, Mathieu Specklin.

Kesaco is a set of libraries and programs aiming at applications of mathematical modeling in clinical oncology. It features:

- A library of specialized mathematical model describing the growth of different types of cancers (secondary tumors in the lung, gliomas).
- A set of programs useful to validate mathematical models (compute the various behavior they can produce) and to build databases of numerical simulations.
- Segmentation and registration routines to use medical images directly in our numerical codes.
- Calibration methods to recover the parameters of the models using sequences of medical images. Three techniques are implemented (a genetic algorithm, a technique based on reduced order models, a sensitivity technique).
All these routines are adapted to run on a MP architecture. The webpage may be found at http://www.math.u-bordeaux1.fr/~osaut/pages/kesaco.html.

- Version: 0.1
- Keywords: Modélisation and numerical simulations
- APP: En cours
- Type of human computer interaction: console
- OS/Middleware: Platform developed on Mac OS X architecture.
- Required library or software: eLYSe, Insight Toolkit (http://www.itk.org)
- Programming language: C++
- Documentation: doxygen.

5.3. NaSCar

**Participant:** Michel Bergmann [correspondant].

This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam’s type. The code is written in C language and use Petsc (http://www.mcs.anl.gov/petsc/petsc-as/) library for the resolution of large linear systems in parallel.

NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Version: 1
- Keywords: numerical analyse, fluid mechanics, langage C, PETSc
- Software benefit: simulate a flow around a deformable obstacle, moving into a fluid.
- APP: En cours
- Patent: non
- Type of human computer interaction: human for the moment
- OS/Middleware: unix, linux, mac os
- Required library or software: PETSc item Programming language: C
- Documentation: in progress

5.4. S-MPI-2D-3D

**Participants:** Charles-Henri Bruneau [correspondant], Khodor Khadra.

The software NS-MPI-2D-3D is a numerical platform devoted to the computation of the incompressible flow around bodies in two or three dimensions modelled by Stokes, Navier-Stokes or Oldroyd-B equations. It is based on finite differences or finite volumes approximations on cartesian grid using the volume penalization method to handle the obstacles. The resolution is achieved by means of the multigrid method. Dirichlet, periodic or artificial boundary conditions are implemented to solve various problems in closed or open domains.

- Version: 3
- Keywords: Numerical simulation of incompressible flows,
- Type of human computer interaction: console
- OS/Middleware: unix, linux, Mac OS X item Programming language: Fortran 95 and MPI
- Documentation: included
5.5. Other MC2 codes

- Penalization techniques on cartesian grids to solve incompressible Navier-Stokes equations
  - **Vortex**: sequential, Vortex In-Cell (VIC) scheme: hybrid vortex methods based on the combination of Lagrangian mesh-free schemes and Eulerian grid based schemes on the same flow region.
  - Unstructured body fitted meshes
  - **Richards**: 2D Unstructured finite element code, implicit solver, sequential, to solve the transport-diffusion equations through a porous media including tidal forcing and mechanisms of diagenesis.
  - development inside **FluidBox** software in collaboration with **BACCHUS**, 2D-3D unstructured meshes, Stabilized Finite Elements method (SUPG), RANS turbulence model, parallel: Domain Decomposition and MPI.

- Immersed boundary techniques for:
  - **Compressible flows**: 2D-3D finite volume scheme for compressible Euler equations with solid obstacles on cartesian grids. 3D code parallelized with MPI
  - **Elliptic problems**: 2D-3D finite difference scheme for elliptic interface problems, parallelized with PETSc
  - Electropermeabilization: 2D finite difference scheme, parallelized with PETSc to simulate the electropermeabilization of biological cells
MICMAC Project-Team (section vide)
5. Software

5.1. MAXW-DGTD

Participants: Stéphane Lanteri [correspondant], Loula Fezoui.

MAXW-DGTD is a software suite for the simulation of time domain electromagnetic wave propagation. It implements a solution method for the Maxwell equations in the time domain. MAXW-DGTD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes [14]. Within each element of the mesh, the components of the electromagnetic field are approximated by arbitrary high order nodal polynomial interpolation method. This discontinuous Galerkin method combines a centered scheme for the evaluation of numerical fluxes at a face shared by two neighboring elements, with an explicit Leap-Frog time scheme. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with message passing programming using the MPI standard. Besides, a peripheral version of the software has been recently developed which is able to exploit the processing capabilities of a hybrid parallel computing system comprising multicores CPU and GPU nodes [27].

- AMS: AMS 35L50, AMS 35Q60, AMS 35Q61, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational electromagnetics, Maxwell equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface), CUDA
- Programming language: Fortran 77/95

5.2. MAXW-DGFD

Participant: Stéphane Lanteri [correspondant].

MAXW-DGFD is a software suite for the simulation of time harmonic electromagnetic wave propagation. It implements a solution method for the Maxwell equations in the frequency domain. MAXW-DGFD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes. Within each element of the mesh, the components of the electromagnetic field are approximated by arbitrary high order nodal polynomial interpolation method. The resolution of the sparse, complex coefficients, linear systems resulting from the discontinuous Galerkin formulation is performed by a hybrid iterative/direct solver whose design is based on domain decomposition principles. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with a message passing programming using the MPI standard. Some recent achievements have been the implementation of non-uniform order DG method in the 2D case [18] and of a new hybridizable discontinuous Galerkin (HDG) formulation also in the 2D case [22].

- AMS: AMS 35L50, AMS 35Q60, AMS 35Q61, AMS 65N08, AMS 65N30, AMS 65M60
- Keywords: Computational electromagnetics, Maxwell equations, discontinuous Galerkin, tetrahedral mesh.
- OS/Middleware: Linux
- Required library or software: MPI (Message Passing Interface)
- Programming language: Fortran 77/95

5.3. SISMO-DGTD

Participants: Nathalie Glinsky [correspondant], Stéphane Lanteri.
SISMO-DGTD is a software for the simulation of time domain seismic wave propagation. It implements a solution method for the velocity-stress equations in the time domain. SISMO-DGTD is based on a discontinuous Galerkin method formulated on unstructured triangular (2D case) or tetrahedral (3D case) meshes [5]. Within each element of the mesh, the components of the electromagnetic field are approximated by an arbitrary high order nodal polynomial interpolation method. This discontinuous Galerkin method combines a centered scheme for the evaluation of numerical fluxes at a face shared by two neighboring elements, with an explicit Leap-Frog time scheme. The software and the underlying algorithms are adapted to distributed memory parallel computing platforms thanks to a parallelization strategy that combines a partitioning of the computational domain with a message passing programming using the MPI standard.

AMS: AMS 35L50, AMS 35Q74, AMS 35Q86, AMS 65N08, AMS 65N30, AMS 65M60
Keywords: Computational geoseismics, elastodynamic equations, discontinuous Galerkin, tetrahedral mesh.
OS/Middleware: Linux
Required library or software: MPI (Message Passing Interface)
Programming language: Fortran 77/95

5.4. NUM3SIS
Participants: Nora Aissiouene, Thibaud Kloczko [SED team], Régis Duigneau [OPALE project-team], Thibaud Kloczko [SED team], Stéphane Lanteri, Julien Wintz [SED team].

NUM3SIS http://num3sis.inria.fr is a modular platform devoted to scientific computing and numerical simulation. It is designed to handle complex multidisciplinary simulations involving several fields such as Computational Fluid Dynamics (CFD), Computational Structural Mechanic (CSM) and Computational ElectroMagnetics (CEM). In this context, the platform provides a comprehensive framework for engineers and researchers that speeds up implementation of new models and algorithms. From a software engineering point of view, num3sis specializes and extends some layers of the meta-platform dtk, especially its core and composition layers. The core layer enables the user to define generic concepts used for numerical simulation such as mesh or finite-volume schemes which are then implemented through a set of plugins. The composition layer provides a visual programming framework that wraps these concepts inside graphical items, nodes. These nodes can then be connected to each other to define data flows (or compositions) corresponding to the solution of scientific problems. NUM3SIS provides a highly flexible, re-usable and efficient approach to develop new computational scenarios and takes advantage of existing tools. The team participates to the development of the NUM3SIS platform through the adaptation and integration of the MAXW-DGTD simulation software. This work is being carried out with the support of two engineers in the framework of an ADT (Action de Développement Technologique) program.

5.5. Medical Image Extractor
Participants: Stéphane Lanteri, Julien Wintz [SED team].

Medical Image Extractor http://num3sis.inria.fr/software/apps/extractor provides functionalities needed to extract meshes from labeled MR or PET-CT medical images. It puts the emphasis on consistence, by generating both boundary surfaces, and volume meshes for each label (ideally identifying a tissue) of the input image, using the very same tetrahedrization. As this process requires user interaction, images and meshes are visualized together with tools allowing navigation and both easy and accurate refinement of the generated meshes, that can then be exported to serve as an input for other tools, within a multidisciplinary software toolchain. Using both DTK http://dtk.inria.fr and NUM3SIS SDKs, Medical Image Extractor comes within NUM3SIS’ framework. Using cutting edge research algorithms developed by different teams at Inria, spread among different research topics, namely, visualization algorithms from medical image processing, meshing algorithms from algorithmic geometry, it illustrates the possibility to bridge the gap between software that come from different communities, in an innovative and highly non invasive development fashion.

3 Service d'Experimentation et de Développement
5. Software

5.1. SAMSON

A major objective of NANO-D is to try and integrate a variety of adaptive algorithms into a unified framework. As a result, NANO-D is developing SAMSON (Software for Adaptive Modeling and Simulation Of Nanosystems), a software platform aimed at including all developments from the group, in particular those described below.

The objective is to make SAMSON a generic application for computer-aided design of nanosystems, similar to existing applications for macrosystem prototyping (CATIA, SolidWorks, etc.).

The current architecture of SAMSON is visible in Figure 6. The code is organized into four main parts: a) the Base (in which “Core” contains, in particular, the heart of the adaptive algorithms: signaling mechanisms specifically designed for SAMSON), b) the Software Development Kit (SDK: a subset of the base that will be provided to module developers), c) Modules, and d) the SAMSON application itself.

Similar to the concept of Mathematica toolboxes, for example, the goal has been to make it possible to personalize the user interface of SAMSON for potentially many distinct applications. For example, we may want to personalize the interface of SAMSON for crystallography, drug design, protein folding, electronics, material science, nano-engineering, etc., by loading different modules at startup, depending on the user application domain.

Figure 6. SAMSON’s architecture.
OPALE Project-Team

5. Software

5.1. NUM3SIS

Participants: Régis Duvigneau [correspondant], Nora Aïssiouene, Babett Lekouta.

NUM3SIS (http://num3sis.inria.fr) is a modular platform devoted to scientific computing and numerical simulation. It is not restricted to a particular application field, but is designed to host complex multidisciplinary simulations. Main application fields are currently Computational Fluid Dynamics (CFD), Computational Electro-Magnetics (CEM, in collaboration with Nachos Project-Team) and pedestrian traffic simulation.

The most important concept in NUM3SIS is the concept of node. It is a visual wrapper around derivatives of fundamental concepts such as data, algorithm or viewer. Atomic nodes are provided for convenience in order to manipulate computational data (such as grids or fields), apply computational methods (such as the building of a finite-element matrix or the construction of a finite-volume flux) and visualize computational results (such as vector or tensor fields, on a screen or in an immersive space). For a given abstract node, different implementations can be found, each of them being embedded in a plugin system that is managed by a factory.

The second important concept in NUM3SIS is the concept of composition. It consists of the algorithmic pipeline used to link the nodes together. The use of these two concepts, composition and nodes, provides a highly flexible, re-usable and efficient approach to develop new computational scenarios and take benefit from already existing tools. This is a great advantage with respect to classical monolithic softwares commonly used in these fields.

This work is being carried out with the support of two engineers in the framework of an ADT (Action de Développement Technologique) program.

5.2. FAMOSA

Participant: Régis Duvigneau [correspondant].

Opale team is developing the software platform FAMOSA (C++), that is devoted to multidisciplinary design optimization in engineering. It integrates the following components:

- an optimization library composed of various algorithms: several descent methods from steepest-descent method to quasi-Newton BFGS method (deterministic, smooth), the Multi-directional Search Algorithm (deterministic, noisy), the Covariance Matrix Adaption Evolution Strategy (semi-stochastic, multi-modal) and the Efficient Global Optimization method (deterministic, multi-modal).
- It also contains the Pareto Archived Evolution Strategy to solve multi-objective optimization problems;
- an evaluation library managing the performance estimation process (communication with external simulation tools);
- a metamodel library that contains tools to build a database and kriging models that are used to approximate the objective function for different purposes;
- a scenario library that allows to use the previous components to achieve various tasks:
  - Construct a design of experiments;
  - Construct a metamodel;
  - Find the design that minimizes a cost functional;
  - Find the Pareto front for two cost functionals;
  - Play a Nash game to find the equilibrium between two criteria;
  - Apply a multiple gradient descent strategy to improve simultaneously two criteria.
The FAMOSA platform is employed by Opale Project-Team to test its methodological developments in multidisciplinary design optimization (MDO). The platform is also used by the Fluid Mechanics Laboratory at Ecole Centrale de Nantes and by the K-Epsilon company (http://www.k-epsilon.com) for hydrodynamic design applications. Moreover, it is presently tested by Peugeot Automotive industry for external aerodynamic design purpose.

5.3. Plugins for AXEL

Participants: Régis Duvigneau [correspondent], Louis Blanchard.

Opale team is developing plugins in the framework of the algebraic modeler Axel, in collaboration with GALAAD team. These developments correspond to two research axes:

- methods for isogeometric analysis and design. In particular, two simulation tools for heat conduction and compressible flows have been implemented, in conjunction with some deterministic and semi-stochastic optimization algorithms for optimum-shape design;
- methods for geometrical modeling of bow shapes for trawler ships.

5.4. Integration platform for multidiscipline optimization applications

Participants: Toan Nguyen, Laurentiu Trifan.

A prototype software integration platform is developed and tested for multidiscipline optimization applications. It is based on a workflow management system called YAWL (http://www.yawlfoundation.org). The goal is to design, develop and assess high-performance distributed scientific workflows featuring resilience, i.e., fault-tolerance and exception-handling capabilities. The platform is used to experiment new resilience algorithms, including monitoring and management of application-level errors. Errors include time-outs and out of bounds data values. They can be added and modified by the users. The platform is tested against use-cases provided by the industry partners in the OMD2 project supported by the French Agence Nationale de la Recherche. For example, an optimization of a car air-conditioning pipe was implemented and deployed on the Grid5000 infrastructure. It also takes into account run-time errors related to resource consumption, e.g., memory overflow, to automatically and dynamically relocate the applications tasks involved on the various clusters. This work is part of Laurentiu Trifan’s PhD thesis that is to be defended in 2013. (See Fig. 1.)

![Figure 1: Testcase deployment on the Grid5000 infrastructure.](image)
5. Software

5.1. Introduction

We are led to develop two types of software. The first one is prototype softwares: various softwares are developed in the framework of specific research contracts (and sometimes sold to the contractor) or during PhD theses. They may be also contributions to already existing softwares developed by other institutions such as CEA, ONERA or EDF. The second category is an advanced software which are intended to be developed, enriched and maintained over longer periods. Such software is devoted to help us for our research and/or promote our research. We have chosen to present here only our advanced software.

5.2. XLIFE++

XLIFE++ is a new Finite Element library in C++ based on philosophy of the previous library MELINA in Fortran but with new capabilities (boundary element, discontinuous Galerkin methods, more integrated tools (in particular mesh tools) and high performance computing skills (multithread and GPU computation). It is licensed under LGPL and it is developped in the context of the european project SIMPOSIUM (FP7/ICT, leader CEA/LIST, from september 2011 to august 2014). There are also academic partners: Irmar-univ. Rennes and Lama-univ. Paris-Est. In 2012, all development tools have been set up: versioning using Git, repository on Inria-Gforge, compiling and installing tools using Cmake, documentation in TeX and using Doxygen), test processing. All fundamentals library have been developed and checked (String, Function, Messages, Matrix, Vector, ...) and major libraries are done: geometry (Mesh description and tools), space,form, operators to deal with variational descriptions of PDE problem, finiteElements describing all finite elements description, term wich deals with sparse matrix representation of linear or bilinear forms involved in variational problems and finally the solvers library. A first version of the library should be published soon.
5. Software

5.1. AIRONUM

**Participant:** Alain Dervieux [correspondant].

AIRONUM is an experimental software that solves the unsteady compressible Navier-Stokes equations with $k - \varepsilon$, LES-VMS and hybrid turbulence modelling on parallel platforms with Mpi as parallel programming concept. The mesh model is unstructured tetrahedrization, with possible mesh motion. See also [http://www-sop.inria.fr/tropics/aironum](http://www-sop.inria.fr/tropics/aironum)

- **Version:** v 1.0
- **Programming language:** Fortran95 (mostly). About 100,000 lines.

AIRONUM was developed by Inria and university of Montpellier. It is used by Inria, university of Montpellier and university of Pisa (I). AIRONUM is used as an experimental platform for:

- Numerical approximation of compressible flows, such as upwind mixed element volume approximation with superconvergence on regular meshes.
- Numerical solution algorithms for the implicit time advancing of the compressible Navier-Stokes equations, such as parallel scalable deflated additive Schwarz algorithms.
- Turbulence modelling such as the Variational Multiscale Large eddy Simulation and its hybridization with RANS statistical models.

5.2. TAPENADE

**Participants:** Laurent Hascoët [correspondant], Valérie Pascual.

TAPENADE is an Automatic Differentiation tool that transforms an original program into a new program that computes derivatives of the original program. Automatic Differentiation produces analytical derivatives, that are exact up to machine precision. Adjoint-mode AD can compute gradients at a cost which is independent from the number of input variables. TAPENADE accepts source programs written in Fortran77, Fortran90, or C. It provides differentiation in the following modes: tangent, vector tangent, and adjoint. Documentation is provided on the web site of the research team and as the Inria technical report RT-0300. TAPENADE runs under most operating systems and requires installation of Java jdk1.6 or upward. See also [http://www-sop.inria.fr/tropics/](http://www-sop.inria.fr/tropics/)

- **Version:** v3.6, r4343, February 2012
- **ACM:** D.3.4 Compilers; G.1.0 Numerical algorithms; G.1.4 Automatic differentiation; I.1.2 Analysis of algorithms
- **AMS:** 65K10; 68N20
- **APP:** IDDN.FR.001.040038.002.S.P.2002.000.10600
- **Keywords:** automatic differentiation, adjoint, gradient, optimisation, inverse problems, static analysis, data-flow analysis, compilation
- **Programming language:** Java

TAPENADE implements the results of our research about models and static analyses for AD. TAPENADE can be downloaded and installe on most architectures. Alternatively, it can be used as a web server. TAPENADE differentiates computer programs according to the model described in section 3.1 and in [19] Higher-order derivatives can be obtained through repeated application of tangent AD on tangent- and/or adjoint-mode AD.
TAPENADE performs sophisticated data-flow analysis, flow-sensitive and context-sensitive, on the complete source program to produce an efficient differentiated code. Analyses include Type-Checking, Read-Write analysis, and Pointer analysis. AD-specific analysis include:

- **Activity analysis**: Detects variables whose derivative is either null or useless, to reduce the number of derivative instructions.
- **Adjoint Liveness analysis**: Detects the source statements that are dead code for the computation of derivatives.
- **TBR analysis**: In adjoint-mode AD, reduces the set of source variables that need to be recovered.

TAPENADE is not open-source. Academic usage is free. Industrial or commercial usage require a paying license, as detailed on the team’s web page. The software has been downloaded several hundred times, and the web tool served several thousands of true connections (not counting robots). The tapenade-users mailing list is over one hundred registered users.
**SIMPAF Project-Team**

5. Software

5.1. ns2ddv-M

**Participants:** Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)].

Incompressible Navier-Stokes, Variable Density, Rayleigh-Taylor Instability The NS2DDV-M code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. This original approach for variable density flows is described in [56]. The NS2DDV-M code will be available on the SIMPAF team web page before the end of 2011.

Here is the self-assessment of the team effort following the grid provided by Inria (see : http://www.inria.fr/institut/organisation/instances/commission-d-evaluation): A3, SO3-up4, SM2-up3, EM3, SDL4, DA1, CD4, MS4, TPM4.

Software web site : http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html

5.2. ns2ddv-C++

**Participants:** Caterina Calgaro [correspondant (Univ. Lille 1)], Emmanuel Creusé [correspondant (Univ. Lille 1)], Thierry Goudon.

Incompressible Navier-Stokes, Variable Density, Kazhikhov-Smagulov model, Rayleigh-Taylor Instability, avalanches phenomena The NS2DVD-C++ code is based on a hybrid method coupling FV and FE approaches for solving the variable density Navier-Stokes equation in dimension 2. The code is developed around the GetFem++ and the Bamg softwares. It allows in particular mesh refinement strategies so that very relevant simulations can be reached (as the falling droplet with very high density ratios, see for example [54]. The current version of the code consider the additional terms in the Kazhikhov-Smagulov model.

Webpage : http://math.univ-lille1.fr/~simpaf/SITE-NS2DDV

Here is the self-assessment of the team effort following the grid provided by Inria (see : http://www.inria.fr/institut/organisation/instances/commission-d-evaluation): A1, SO3-up4, SM1, EM2, SDL1, DA1, CD4, MS4, TPM1.

5.3. RTcodes

**Participants:** Pauline Lafitte [correspondant (ECP)], Jean-François Coulombel [(CNRS & Univ. Nantes)], Christophe Besse [(Univ. Lille 1)], Thierry Goudon [(Inria)], Giovanni Samaey [(KU Leuven)].

Radiative Transfer, Radiative shocks, AP schemes

We have developed a set of numerical codes, written in Scilab, to compute the solutions of the system coupling the Euler equations to the radiation through energy exchanges, in the non equilibrium regime. This covers several situations in the hierarchy of asymptotic problems. The code treats the one-dimensional framework. In particular the code can be used to investigate radiative shocks profiles. The main advantage of our numerical codes is that they do not require any refinement near the singularities. The numerical tests show a very good agreement with the theoretical predictions. See reference [27].

Here is the self-assessment of the team effort following the grid provided by Inria (see : http://www.inria.fr/institut/organisation/instances/commission-d-evaluation): A2, SO3, SM2, EM1, SDL1.
5.4. FPcodes

**Participants:** Pauline Lafitte [correspondant (ECP)], Thierry Goudon [(Inria)], Benjamin Boutin [(Univ. Rennes)].

Fluid-Particles flows, Gravity driven flows, AP schemes

We have developed a numerical code, written in Scilab, to compute the solutions of the two-phase flows equations describing particles interacting with a fluid through friction forces. The code treats one-dimensional situation and is well adapted to describe gravity driven flows in either bubbling or flowing regimes. In particular, it can be used to describe the evolution of pollutants in the atmosphere. The numerical strategy, based on a asymptotic-based scheme, is described in details in [57].

Here is the self-assessment of the team effort following the grid provided by Inria (see: http://www.inria.fr/institut/organisation/instances/commission-d-evaluation): A2, SO3, SM2, EM1, SDL1.

5.5. CLAToolBox

**Participant:** Christophe Besse [correspondant].

Absorbant boundary conditions, Schrödinger equation

As a byproduct of the review paper [45], a user-friendly interface is offered to trial and compare various numerical methods to solve the 1D Schrödinger equation with absorbant boundary conditions. We also mention [50] for a numerical investigation of blow-up phenomena in the nonlinear Schrödinger equation.

5.6. SPARCS

**Participant:** Christophe Besse.

Vlasov-Poisson system, Euler-Poisson system. Back-Trajectory method

SPARCS is the code developed by Thales Alenia Space for the simulation of the charge phenomena the spacecrafts are subject to. The current version of the code, according to the PhD thesis of O. Chanrion and M. Chaney-Yook performed in collaboration with the team Caiman at Sophia Antipolis, is specialized to geostationary atmospheres. The model consists in the stationary Vlasov-Poisson system, but where instationary effects are taken into account with the boundary condition for the electric field. We participate, in particular through the post doc of N. Vauchelet, to the elaboration of an improved version of the code which includes parallization optimized procedures, the modelling of the natural difference of potential between different dielectric surfaces of the spacecraft, as well as the possible presence of devices emitting charged particles.

5.7. Code-Carmel3D

**Participant:** Emmanuel Creusé [correspondant (Univ. Lille 1)].

This numerical code, developed in collaboration between EDF R&D and Lille 1 University, is devoted to the electromagnetic fields computation by the use of finite element methods. This code allows in particular to perform nondestructive control by the use of Foucault currents in steam generator pipes, and should be soon coupled with the thermal simulation of Code-Aster. Code-Carmel3D uses the Salomé platform (mesh-generator and post-processing) and Open Turns (uncertainties computation). It will consequently allow to solve multi-physics problems, both for the temporal and harmonic formulations.

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1 http://math.univ-lille1.fr/~besse/site/recherche/logiciels/index.html
5. Software

5.1. RARL2

Participant: Martine Olivi [corresponding participant].

Status: Currently under development. A stable version is maintained.

This software is developed in collaboration with Jean-Paul Marmorat (Centre de mathématiques appliquées (CMA), École des Mines de Paris).

RARL2 (Réalisation interne et Approximation Rationnelle L2) is a software for rational approximation (see section 3.3.2.2) http://www-sop.inria.fr/apics/RARL2/rarl2-eng.html.

The software RARL2 computes, from a given matrix-valued function in $\mathbb{H}^{m \times l}$, a local best rational approximant in the $L^2$ norm, which is stable and of prescribed McMillan degree (see section 3.3.2.2). It was initially developed in the context of linear (discrete-time) system theory and makes an heavy use of the classical concepts in this field. The matrix-valued function to be approximated can be viewed as the transfer function of a multivariable discrete-time stable system. RARL2 takes as input either:

- its internal realization,
- its first $N$ Fourier coefficients,
- discretized (uniformly distributed) values on the circle. In this case, a least-square criterion is used instead of the $L^2$ norm.

It thus performs model reduction in case 1) and 2) and frequency data identification in case 3). In the case of band-limited frequency data, it could be necessary to infer the behavior of the system outside the bandwidth before performing rational approximation (see 3.2.2). An appropriate Moebius transformation allows to use the software for continuous-time systems as well.

The method is a steepest-descent algorithm. A parametrization of MIMO systems is used, which ensures that the stability constraint on the approximant is met. The implementation, in matlab, is based on state-space representations.

The number of local minima can be rather high so that the choice of an initial point for the optimization can play a crucial role. Two methods can be used: 1) An initialization with a best Hankel approximant. 2) An iterative research strategy on the degree of the local minima, similar in principle to that of Rarl2, increases the chance of obtaining the absolute minimum by generating, in a structured manner, several initial conditions.

RARL2 performs the rational approximation step in our applications to filter identification (see section 4.3) as well as sources or cracks recovery (see section 4.2). It was released to the universities of Delft, Maastricht, Cork and Brussels. The parametrization embodied in RARL2 was also used for a multi-objective control synthesis problem provided by ESTEC-ESA, The Netherlands. An extension of the software to the case of triple poles approximants is now available. It provides satisfactory results in the source recovery problem and it is used by FindSources3D (see section 5.6).

5.2. RGC

Participant: Fabien Seyfert [corresponding participant].

Status: A stable version is maintained.

This software is developed in collaboration with Jean-Paul Marmorat (Centre de mathématiques appliquées (CMA), École des Mines de Paris).
The identification of filters modelled by an electrical circuit that was developed by the team (see section 4.3) led us to compute the electrical parameters of the underlying filter. This means finding a particular realization \((A,B,C,D)\) of the model given by the rational approximation step. This 4-tuple must satisfy constraints that come from the geometry of the equivalent electrical network and translate into some of the coefficients in \((A,B,C,D)\) being zero. Among the different geometries of coupling, there is one called “the arrow form” [53] which is of particular interest since it is unique for a given transfer function and is easily computed. The computation of this realization is the first step of RGC. Subsequently, if the target realization is not in arrow form, one can nevertheless show that it can be deduced from the arrow-form by a complex-orthogonal change of basis. In this case, RGC starts a local optimization procedure that reduces the distance between the arrow form and the target, using successive orthogonal transformations. This optimization problem on the group of orthogonal matrices is non-convex and has many local and global minima. In fact, there is not even uniqueness of the filter realization for a given geometry. Moreover, it is often relevant to know all solutions of the problem, because the designer is not even sure, in many cases, which one is being handled. The assumptions on the reciprocal influence of the resonant modes may not be equally well satisfied for all such solutions, hence some of them should be preferred for the design. Today, apart from the particular case where the arrow form is the desired form (this happens frequently up to degree 6) the RGC software provides no guarantee to obtain a single realization that satisfies the prescribed constraints. The software Dedale-HF (see section 5.4), which is the successor of RGC, solves with guarantees this constraint realization problem.

5.3. PRESTO-HF

**Participant**: Fabien Seyfert [corresponding participant].

Status: Currently under development. A stable version is maintained.

PRESTO-HF: a toolbox dedicated to lowpass parameter identification for microwave filters [http://www-sop.inria.fr/apics/personnel/Fabien.Seyfert/Presto_web_page/presto_pres.html](http://www-sop.inria.fr/apics/personnel/Fabien.Seyfert/Presto_web_page/presto_pres.html). In order to allow the industrial transfer of our methods, a Matlab-based toolbox has been developed, dedicated to the problem of identification of low-pass microwave filter parameters. It allows one to run the following algorithmic steps, either individually or in a single shot:

- determination of delay components caused by the access devices (automatic reference plane adjustment),
- automatic determination of an analytic completion, bounded in modulus for each channel,
- rational approximation of fixed McMillan degree,
- determination of a constrained realization.

For the matrix-valued rational approximation step, Presto-HF relies on RARL2 (see section 5.1), a rational approximation engine developed within the team. Constrained realizations are computed by the RGC software. As a toolbox, Presto-HF has a modular structure, which allows one for example to include some building blocks in an already existing software.

The delay compensation algorithm is based on the following strong assumption: far off the passband, one can reasonably expect a good approximation of the rational components of \(S_{11}\) and \(S_{22}\) by the first few terms of their Taylor expansion at infinity, a small degree polynomial in \(1/s\). Using this idea, a sequence of quadratic convex optimization problems are solved, in order to obtain appropriate compensations. In order to check the previous assumption, one has to measure the filter on a larger band, typically three times the pass band.

This toolbox is currently used by Thales Alenia Space in Toulouse, Thales airborn systems and a license agreement has been recently negotiated with TAS-Espagna. XLim (University of Limoges) is a heavy user of Presto-HF among the academic filtering community and some free license agreements are currently being considered with the microwave department of the University of Erlangen (Germany) and the Royal Military College (Kingston, Canada).

5.4. Dedale-HF

**Participant**: Fabien Seyfert [corresponding participant].
Dedale-HF is a software dedicated to solve exhaustively the coupling matrix synthesis problem in reasonable time for the users of the filtering community. For a given coupling topology, the coupling matrix synthesis problem (C.M. problem for short) consists in finding all possible electromagnetic coupling values between resonators that yield a realization of given filter characteristics (see section 6.3). Solving the latter problem is crucial during the design step of a filter in order to derive its physical dimensions as well as during the tuning process where coupling values need to be extracted from frequency measurements (see Figure 3).

Dedale-HF consists in two parts: a database of coupling topologies as well as a dedicated predictor-corrector code. Roughly speaking each reference file of the database contains, for a given coupling topology, the complete solution to the C.M. problem associated to particular filtering characteristics. The latter is then used as a starting point for a predictor-corrector integration method that computes the solution to the C.M. problem of the user, i.e. the one corresponding to user-specified filter characteristics. The reference files are computed off-line using Groebner basis techniques or numerical techniques based on the exploration of a monodromy group. The use of such a continuation technique combined with an efficient implementation of the integrator produces a drastic reduction, by a factor of 20, of the computational time.

Access to the database and integrator code is done via the web on http://www-sop.inria.fr/apics/Dedale/WebPages. The software is free of charge for academic research purposes: a registration is however needed in order to access full functionality. Up to now 90 users have registered world wide (mainly: Europe, U.S.A, Canada and China) and 4000 reference files have been downloaded.

A license of this software has been sold end 2011, to TAS-Espagna to tune filter, with topologies with multiple solutions. The usage of Dedale-HF is here considered together with Presto-HF.

Figure 3. Overall scheme of the design and tuning process of a microwave filter.
5.5. easyFF

**Participant:** Fabien Seyfert.

Status: A stable version is maintained.

This software has been developed by Vincent Lunot (Taiwan Univ.) during his Ph.d. He still continues to maintain it.

EasyFF is a software dedicated to the computation of complex, and in particular multi-band, filtering functions. The software takes as input, specifications on the modulus of the scattering matrix (transmission and rejection), the filter’s order and the number of transmission zeros. The output is an “optimal” filtering characteristic in the sense that it is the solution of an associated min-max Zolotarev problem. Computations are based on a Remez-type algorithm (if transmission zeros are fixed) or on linear programming techniques if transmission zeros are part of the optimization [11].

5.6. FindSources3D

**Participant:** Juliette Leblond [corresponding participant].

Status: Currently under development. A stable version is maintained.

This software is developed in collaboration with Maureen Clerc and Théo Papadopoulo from the Athena EPI, and with Jean-Paul Marmorat (Centre de mathématiques appliquées (CMA), École des Mines de Paris).

FindSources3D is a software dedicated to source recovery for the inverse EEG problem, in 3-layer spherical settings, from pointwise data (see [http://www-sop.inria.fr/apics/FindSources3D/](http://www-sop.inria.fr/apics/FindSources3D/)). Through the algorithm described in [16] and section 4.2, it makes use of the software RARL2 (section 5.1) for the rational approximation step in plane sections. The data transmission preliminary step (“cortical mapping”) is solved using boundary element methods through the software OpenMEEG (its CorticalMapping features) developed by the Athena Team (see [http://www-sop.inria.fr/athena/software/OpenMEEG/](http://www-sop.inria.fr/athena/software/OpenMEEG/)). A first release of FindSources3D is now available, which will be demonstrated and distributed within the medical teams we are in contact with (see Figure 4, CeCILL license, APP version 1.0: IDDN.FR.001.45009.S.A.2009.000.10000).

![Figure 4. Potential values at electrodes on a sphere (scalp), recovered 2 sources (FindSources3D).](image-url)
5.7. Sollya

**Participant:** Sylvain Chevillard [corresponding participant].

**Status:** Currently under development. A stable version is maintained.

This software is developed in collaboration with Christoph Lauter (LIP6) and Mioara Joldeș (Uppsala University, Sweden).

Sollya is an interactive tool where the developers of mathematical floating-point libraries (libm) can experiment before actually developing code. The environment is safe with respect to floating-point errors, *i.e.* the user precisely knows when rounding errors or approximation errors happen, and rigorous bounds are always provided for these errors.

Amongst other features, it offers a fast Remez algorithm for computing polynomial approximations of real functions and also an algorithm for finding good polynomial approximants with floating-point coefficients to any real function. It also provides algorithms for the certification of numerical codes, such as Taylor Models, interval arithmetic or certified supremum norms.

It is available as a free software under the CeCILL-C license at [http://sollya.gforge.inria.fr/](http://sollya.gforge.inria.fr/).
5. Software

5.1. Nonsmooth dynamics: Siconos

Participants: Vincent Acary, Maurice Bremond, Olivier Bonnefon.

In the framework of the European project Siconos, Bipop was the leader of the Work Package 2 (WP2), dedicated to the numerical methods and the software design for nonsmooth dynamical systems. The aim of this work is to provide a common platform for the simulation, modeling, analysis and control of abstract nonsmooth dynamical systems. Besides usual quality attributes for scientific computing software, we want to provide a common framework for various scientific fields, to be able to rely on the existing developments (numerical algorithms, description and modeling software), to support exchanges and comparisons of methods, to disseminate the know-how to other fields of research and industry, and to take into account the diversity of users (end-users, algorithm developers, framework builders) in building expert interfaces in Python and end-user front-end through Scilab.

After the requirement elicitation phase, the Siconos Software project has been divided into 5 work packages which are identified to software products:

1. SICONOS/NUMERICS This library contains a set of numerical algorithms, already well identified, to solve non smooth dynamical systems. This library is written in low-level languages (C,F77) in order to ensure numerical efficiency and the use of standard libraries (Blas, Lapack, ...)

2. SICONOS/KERNEL. This module is an object-oriented structure (C++) for the modeling and the simulation of abstract dynamical systems. It provides the users with a set of classes to describe their nonsmooth dynamical system (dynamical systems, interactions, nonsmooth laws, ...) and to perform a numerical time integration and solving.

3. SICONOS/FRONT-END. This module is mainly an auto-generated wrapper in Python which provides a user-friendly interface to the Siconos libraries. A scilab interface is also provided in the Front-End module.

4. SICONOS/CONTROL. This part is devoted to the implementation of control strategies of non smooth dynamical systems.

5. SICONOS/MULTIBODY. This part is dedicated to the modeling and the simulation of multi-body systems with 3D contacts, impacts and Coulomb’s friction. It uses the Siconos/Kernel as simulation engine but relies on a industrial CAD library (OpenCascade and pythonOCC) to deal with complex body geometries and to compute the contact locations and distances.

Further informations may be found at http://siconos.gforge.inria.fr/

5.2. Humanoid motion analysis and simulation


The HuMaN toolbox offers tools for the modelling, control and analysis of humanoid motion, be it of a robot or a human. It is a C/C++/Scilab/Maple-based set of integrated tools for the generation of dynamical models of articulated bodies with unilateral contact and friction, their simulation with an event-driven integration scheme, their 3D visualization, the computation of stability measures, optimal positions and trajectories, the generation of control laws and observers, the reconstruction of movements from different sensing systems.

5.3. AMELIF

Participants: Pierre-Brice Wieber, François Keith.
The AMELIF framework is an integrative framework that proposes an API for the representation and simulation of virtual scenes including articulated bodies. AMELIF was devised to realize interactive scenario studies with haptic feedback while providing an interface enabling fast and general prototyping of humanoids (avatars or robots). It is entirely developed in C++ and is cross-platform. The framework is articulated around a core library, upon which several modules have been developed for collision detection, dynamic simulation (contact handling in a time stepping scheme), 3D rendering, haptic interaction, posture generation. This framework is developed mostly at the CNRS/AIST UMI JRL, but we started using it in the Bipop team and therefore started contributing actively to its development.

5.4. Optimization

Participant: Claude Lemaréchal.

Essentially two possibilities exist to distribute our optimization software: library programs (say Modulopt codes), communicated either freely or not, depending on what they are used for, and on the other hand specific software, developed for a given application.

The following optimization codes have been developed in the framework of the former Promath project. They are generally available at http://www-rocq.inria.fr/~gilbert/modulopt/; M1QN3 is also distributed under GPL.

5.4.1. Code M1QN3

Optimization without constraints for problems with many variables \((n \geq 10^3)\), has been used for \(n = 10^6\). Technically, uses a limited-memory BFGS algorithm with Wolfe’s line-search (see Chap. 4 of [3] for the terminology).

5.4.2. Code M2QN1

Optimization with simple bound-constraints for (small) problems: \(D\) is a parallelepiped in \(R^n\). Uses BFGS with Wolfe’s line-search and active-set strategy.

5.4.3. Code N1CV2

Minimization without constraints of a convex nonsmooth function by a proximal bundle method (Chap. XV of [10], Chap. 9 of [3]).

5.4.4. Modulopt

In addition to codes such as above, the Modulopt library contains application problems, synthetic or from the real world. It is a field for experimentation, functioning both ways: to assess a new algorithm on a set of test-problems, or to select among several codes one best suited to a given problem.

5.5. MECHE: Simulation of fibrous materials


The software MECHE was essentially developed during the MECHE ADT (2009-2011), for simulating the dynamics of assemblies of thin rods (such as hair), subject to contact and friction. Currently, this software is extensively used by two PhD students (A. Derouet-Jourdan and R. Casati) and continues to be enriched with new rod models and inversion modules. This software combines a panel of well-accepted models for rods (ranging from reduced coordinates to maximal coordinates models, and including models recently developed by some members of the group) with classical as well as innovative schemes for solving the problem of frictional contact (incorporating the most recent results of the group, as well as the new contact solver we published in [8]). The aim of this software is twofold: first, to compare and analyze the performance of nonsmooth schemes for the frictional contact problem, in terms of realism (capture of dry friction, typically), robustness, and computational efficiency. A first study of this kind was conducted in 2010-2011 onto the different rod models that were available in the software. New studies are planned for evaluating further rod models. Second, we believe such a software will help us understand the behavior of a fibrous material (such as hair) through virtual experiments, thanks to which we hope to identify and understand some important
emergent phenomena. A careful validation study against experiments started to be conducted in 2011 in collaboration with physicists from L’Oréal. Once this discrete elements model will be fully validated, our ultimate goal would be to build a continuous macroscopic model for the hair medium relying on nonsmooth laws. The core of this software was transferred to L’Oréal in 2011.
5. Software

5.1. Bocop

Participants: Pierre Martinon [corresponding author], Vincent Grélard, Daphné Giorgi, Frédéric Bonnans.
Web page: http://bocop.org

The Bocop project aims to develop an open-source toolbox for solving optimal control problems, with collaborations with industrial and academic partners. Optimal control (optimization of dynamical systems governed by differential equations) has numerous applications in transportation, energy, process optimization, and biology. The software reuses some packages from the COIN-OR library, in particular the well-known nonlinear programming solver Ipopt, and also features a user-friendly interface.

The project is supported by Inria with the arrival of Vincent Grelard as developer in October 2010, and then Daphné Giorgi in October 2012. The first prototype was released in 2011, and version 1.4 is scheduled for the end of 2012. Bocop was first successfully tested on several academic problems, see [28] available on http://bocop.org. In 2012, several research collaborations were initiated in fields such as bio-reactors for energy production (ref ECC), swimming micro-robots, and quantum control for medical imaging. Bocop was also featured during our participation in the Imatch "Optimisation and Control" in October.

5.2. CollAv

Participants: Hasnaa Zidani [corresponding author], Olivier Bokanowski, Anna Desilles.

This software simulates the evolution of controlled dynamical systems (possibly under uncertainties). The numerical algorithm here is based on HJB or viability approaches, and allows the design of optimal planning strategies (according to a criterion determined by the user: time, energy, …). It also provides conflict resolution and avoidance of collisions with fixed or moving obstacles. So far, the software is used in collaboration with DGA for avoidance collision of UaVs, and by Volkswagen in some studies related to collision avoidance of cars.

5.3. OCOPHyS

Participants: Hasnaa Zidani [corresponding author], Giovanni Granato.

This is a software for optimisation-based controller design for operating in different regimes or modes of operation. The software can be used, for example, to determine the optimal management for hybrid vehicles or hybrid engines with multiple energy sources. However, the methods used in software are still quite general and can be used in many applications.

5.4. BiNoPe-HJ

Participants: Hasnaa Zidani [corresponding author], Olivier Bokanowski, Anna Desilles, Jun-Yi Zhao.
Web page: http://www.ensta-paristech.fr/ zidani/BiNoPe-HJ

This project aims at developing sequential and parallel MPI/openMP C++ solvers for the approximation of Hamilton-Jacobi-Bellman (HJB) equations in a d-dimensional space. The main goal is to provide an HJB solvers that can work in dimension d (limited by the machine’s capacity). The solver outputs can be visualized with Matlab or Paraview (via VTK files).

The development of the HJB Solver has been initiated under a partnership between COMMANDS and the SME HPC-project in the period between December 2009 to November 2011. Currently, it is still maintained and improved by COMMANDS.
In 2012, two versions were released:

- HJB-SEQUENTIAL-REF: sequential version that can run on any machine
- HJB-PARALLEL-REF: parallel version that can run only on multi-core architectures.

5.5. Shoot

**Participant:** Pierre Martinon [corresponding author].

Web page: [http://www.cmap.polytechnique.fr/~martinon/codes.html](http://www.cmap.polytechnique.fr/~martinon/codes.html)

Shoot was designed for the resolution of optimal control problems via indirect methods (necessary conditions, Pontryagin’s Maximum Principle). Such methods transform the original problem into finding a zero of a certain shooting function. The package offers several choices of integrators and solvers, and can handle control discontinuities. Features also include the use of variational equations to compute the Jacobian of the shooting function, as well as homotopy and grid shooting techniques for easier initialization.
5. Software

5.1. Simulation of viscous fluid-structure interactions

Participants: Takeo Takahashi [correspondant], Jean-François Scheid, Jérôme Lohéac.

A number of numerical codes for the simulation for fluids and fluid-structure problems has been developed by the team. These codes are mainly written in MATLAB Software with the use of C++ functions in order to improve the sparse array process of MATLAB. We have focused our attention on 3D simulations which require large CPU time resources as well as large memory storage. In order to solve the 3D Navier-Stokes equations which model the viscous fluid, we have implemented an efficient 3D Stokes sparse solver for MATLAB and a 3D characteristics method to deal with the nonlinearity of Navier-Stokes equations. This year, we have also started to unify our 2D fluid-structure codes (fluid alone, fluid with rigid bodies and fluid with fishes).

Another code has been developed in the case of self-propelled deformable object moving into viscous fluid. Our aim is to build a deformable ball which could swim in a viscous fluid. In order to do this we have started a collaboration with a team from the CRAN (Research Centre for Automatic Control). This software solves numerically 3D Stokes equations using finite elements methods. The source code is written for use with MATLAB thanks to a C++ library developped by ALICE.

- Version: v0.5
- Programming language: MATLABc++

5.2. Fish locomotion in perfect fluids with potential flow

Participants: Alexandre Munnier [correspondant], Marc Fuentes, Bruno Pinçon.

SOLEIL is a Matlab suite to simulate the self-propelled swimming motion of a single 3D swimer immersed in a potential flow. The swimmer is modeled as a shape-changing body whose deformations can be either prescribed as a function of time (simulation of the direct swimming problem) or computed in such a way that the swimmer reaches a prescribed location (control problem). For given deformations, the hydrodynamical forces exerted by the fluid on the swimmer are expressed as solutions of 2D integral equations on the swimmer’s surface, numerically solved by means of a collocation method.

SOLEIL is free, distributed under licence GPL v3. More details are available on the project web page http://soleil.gforge.inria.fr/.

The next step of SOLEIL (under progress) is to take into account a fluid whose flow is governed by Stokes equations.

- Version: 0.1
- Programming language: Matlab/C++
5. Software

5.1. OreModules

**Participants:** Alban Quadrat [correspondent], Daniel Robertz [Univ. Aachen], Frédéric Chyzak [Inria Rocquencourt, Algorithms Project].

The `OreModules` package [88], based on the commercial Maple package Ore-algebra [89], is dedicated to the study of linear multidimensional systems defined over certain Ore algebras of functional operators (e.g., ordinary or partial differential systems, time-delay systems, discrete systems) and their applications in mathematical systems theory, control theory and mathematical physics. `OreModules` is original because it combines the recent developments of the Gröbner bases over some noncommutative polynomial rings [97], [99] and new algorithms of algebraic analysis in order to effectively check classical properties of module theory (e.g., existence of a non-trivial torsion submodule, torsion-freeness, reflexiveness, projectiveness, stably freeness, freeness), it gives their system-theoretical interpretations (existence of autonomous elements or successive parametrizations, existence of minimal/injective parametrizations or Bézout equations) [102], [101], [87] and it computes important tools of homological algebra (e.g., (minimal) free resolutions, split exact sequences, extension functors, projective or Krull dimensions, Hilbert power series). The abstract language of homological algebra used in the algebraic analysis approach carries over to the implementations in `OreModules`: up to the choice of the domain of functional operators which occurs in a given system, all algorithms are stated and implemented in sufficient generality such that linear systems defined over the Ore algebras developed in the Ore-algebra package are covered at the same time. Applications of the `OreModules` package to mathematical systems theory, control theory and mathematical physics are illustrated in a large library of examples. The binary of the package is freely available at http://wwwb.math.rwth-aachen.de/OreModules/.

5.2. Stafford

**Participants:** Alban Quadrat [correspondent], Daniel Robertz [Univ. Aachen].

The `Stafford` package of `OreModules` [88] contains an implementation of two constructive versions of Stafford’s famous but difficult theorem [114] stating that every ideal over the Weyl algebra $A_n(k)$ (resp., $B_n(k)$) of partial differential operators with polynomial (resp., rational) coefficients over a field $k$ of characteristic 0 (e.g., $k = \mathbb{Q}, \mathbb{R}$) can be generated by two generators. Based on this implementation and algorithmic results developed in [109] by the authors of the package, two algorithms which compute bases of free modules over the Weyl algebras $A_n(\mathbb{Q})$ and $B_n(\mathbb{Q})$ have been implemented. The rest of Stafford’s results developed in [114] have recently been made constructive in [112] (e.g., computation of unimodular elements, decomposition of modules, Serre’s splitting-off theorem, Stafford’s reduction, Bass’ cancellation theorem, minimal number of generators) and implemented in the `Stafford` package. The development of the `Stafford` package was motivated by applications to linear systems of partial differential equations with polynomial or rational coefficients (e.g., computation of injective parametrization, Monge problem, differential flatness, the reduction and decomposition problems and Serre’s reduction problem). To our knowledge, the `Stafford` package is the only implementation of Stafford’s theorems nowadays available. The binary of the package is freely available at http://wwwb.math.rwth-aachen.de/OreModules/.

5.3. QuillenSuslin

**Participants:** Alban Quadrat [correspondent], Anna Fabiańska [Univ. Aachen].
The QUILLEN-SUSLIN package [93] contains an implementation of the famous Quillen-Suslin theorem [113], [115]. In particular, this implementation allows us to compute bases of free modules over a commutative polynomial ring with coefficients in a field (mainly $\mathbb{Q}$) and in a principal ideal domain (mainly $\mathbb{Z}$). The development of the QUILLEN-SUSLIN package was motivated by different constructive applications of the Quillen-Suslin theorem in multidimensional systems theory [93] (e.g., the Lin-Bose conjectures, the computation of (weakly) left/right/doubly coprime factorizations of rational transfer matrices, the computation of injective parametrizations of flat linear multidimensional systems with constant coefficients, the reduction and decomposition problems, Serre’s reduction problem). To our knowledge, the QUILLEN-SUSLIN package is the only implementation of the Quillen-Suslin theorem nowadays available. The binary of the package is freely available at http://wwwb.math.rwth-aachen.de/QuillenSuslin.

5.4. OreMorphisms

Participants: Alban Quadrat [correspondent], Thomas Cluzeau [ENSIL, Univ. Limoges].

The OREMORPHISMS package [91] of OREMODULES [87] is dedicated to the implementation of homological algebraic tools such as the computations of homomorphisms between two finitely presented modules over certain noncommutative polynomial algebras (Ore algebras), of kernel, coimage, image and cokernel of homomorphisms, Galois transformations of linear multidimensional systems and idempotents of endomorphism rings. Using the packages STAFFORD and QUILLEN-SUSLIN, the factorization, reduction and decomposition problems can be constructively studied for different classes of linear multidimensional systems. Many linear systems studied in engineering sciences, mathematical physics and control theory have been factorized, reduced and decomposed by means of the OREMORPHISMS package. The binary of the package is freely available at http://www-sop.inria.fr/members/Alban.Quadrat/OreMorphisms/index.html.

5.5. JanetMorphisms

Participants: Alban Quadrat [correspondent], Thomas Cluzeau [ENSIL, Univ. Limoges], Daniel Robertz [Univ. Aachen].

The JANETMORPHISMS package is dedicated to a new mathematic approach to quasilinear systems of partial differential equations (e.g., Burger’s equation, shallow water equations, Euler equations of a compressible fluid) based on algebraic analysis and differential algebra techniques [86]. This package computes symmetries, first integrals of motion, conservation laws, study Riemann invariants... The JANETMORPHISMS package is based on the Janet package (http://wwwb.math.rwth-aachen.de/Janet/).

5.6. PurityFiltration

Participant: Alban Quadrat [correspondent].

The PURITYFILTRATION package, built upon the OREMODULES package, is an implementation of a new effective algorithm obtained in [108] which computes the purity/grade filtration [82], [83] of linear functional systems (e.g., partial differential systems, differential delay systems, difference systems) and equivalent block-triangular matrices. See Section 6.1 . This package is used to compute closed form solutions of over/underdetermined linear partial differential systems which cannot be integrated by the standard computer algebra systems such as Maple and Mathematica. This package will soon be available.

5.7. AbelianSystems

Participants: Alban Quadrat [correspondent], Mohamed Barakat [Univ. Kaiserslautern].
The `ABELIANSYSTEMS` package is an implementation of an algorithm developed in [34] for the computation of the purity/grade filtration [82], [83] in the powerful `homalg` package of GAP 4 dedicated to constructive homological algebra methods, and developed by Barakat (University of Kaiserslautern) and his collaborators (http://homalg.math.rwth-aachen.de/). This package both supersedes the existing `PURITYFILTRATION` package which uses the non-efficient Maple Gröbner basis computation (see Section 5.6.), and the original `homalg` procedure which computes purity filtration by means of time-consuming spectral sequences. Using the `homalg` package philosophy, the `ABELIANSYSTEMS` package can be used for the computation of the purity filtration of objects in different constructive abelian categories such as coherent sheaves over projective schemes as demonstrated in the `homag` package called `Sheaves` (see http://homalg.math.rwth-aachen.de/).

5.8. SystemTheory

**Participants:** Alban Quadrat [correspondent], Thomas Cluzeau [ENSIL, Univ. Limoges], Markus Lange-Hegermann [Univ. Aachen], Mohamed Barakat [Univ. Kaiserslautern].

The `SYSTEMTHEORY` package is a `homalg` based package dedicated to mathematical systems. This package, still in development, will include the algorithms developed in the `OREMODULES` and `OREMORPHISMS` packages. It currently contains an implementation of the `OREMORPHISMS` procedures which handle the decomposition problem aiming at decomposing a module/system into direct sums of submodules/subsystems, and Serre’s reduction problem aiming at finding an equivalent system defined by fewer unknowns and fewer equations.

5.9. YALTA

**Participants:** David Avanessov [correspondent], Catherine Bonnet, André Fioravanti [UNICAMP].

The `YALTA` package is dedicated to the study of classical and fractional systems with delay in the frequency-domain. Its objective is to provide basic but important information such as, for instance, the position of the neutral chains of poles and unstable poles, as well as the root locus with respect to the delay of the system. The corresponding algorithms are based on recent theoretical results (see, for instance, [84] and [95]) and on classical continuation methods exploiting the particularities of the problem [96], [14]. We have included this year a Pade2 approximation scheme as well as $H_{\infty}$-stability properties. The package is freely available at http://team.inria.fr/disco/fr/software/.
5. Software

5.1. IRHD

We developed a first version of a software for reconstruction of corrupted and damaged images, named IRHD (for Image Reconstruction via Hypoelliptic Diffusion). One of the main features of the algorithm on which the software is based is that we don’t use any information about the location and character of the corrupted places; this allows us to work with real non-academic images. Another important advantage is that this method is massively parallelizable; this allows to work with sufficiently large images. Theoretical background of the presented method is based on the model of geometry of vision due to Petitot, Citti and Sarti. The main step is numerical solution of the equation of 3D hypoelliptic diffusion. IRHD is based on Fortran. Alexey Remizov is in charge with the development of the software, in collaboration with Ugo Boscain and Jean-Paul Gauthier.
MAXPLUS Project-Team

5. Software

5.1. Boîte à outil Maxplus de SCILAB/Maxplus toolbox of Scilab

Trois chercheurs du groupe (S. Gaubert, J.-P. Quadrat, et G. Cohen) ont développé (à partir d’une première version réalisée par M. Mc Gettrick) la boîte à outils Maxplus de Scilab, qui est téléchargeable librement parmi les contributions du site Scilab, et qui est maintenant intégrée par défaut dans Scicoslab. Cette boîte à outils implémente l’ensemble du calcul numérique linéaire max-plus, elle comprend en particulier le stockage creux des matrices, et des algorithmes efficaces pour le calcul de la valeur propre basées sur les itérations sur les politiques. Elle a été utilisées par plusieurs chercheurs, voir notamment [70], [134]. Il faut aussi noter que le groupe de L. Hardouin, du LISA/Istia, a complété la boîte à outils Maxplus en interfaçant leur propre librairie C++, qui permet le calcul des séries de transfert de graphes d’événements temporisés.

English version

Three researchers of the team (S. Gaubert, J.-P. Quadrat, and G. Cohen, building on a preliminary version of M. McGettrick) have developed and released the Maxplus toolbox of Scilab, which is freely available among the contributions on the Scilab web site, and which is now included by default in Scicoslab. It implements all basic linear algebra functionalities, with a special attention to large sparse matrices, including efficient algorithms for eigenvalue computation based on policy iteration. The software has been used by several researchers in their work, including [70], [134]. It should be noted that the team of L. Hardouin, from LISA/Istia, has completed the toolbox by interfacing their own C++ library computing the transfer series of a timed event graph.

5.2. Itérations sur les politiques pour les jeux stochastiques à somme nulle/Policy iterations for zero sum stochastic games

L’algorithme d’itérations sur les politiques pour les jeux stochastiques à somme nulle pour le cas de paiements ergodiques (gain moyen par unité de temps), et dégénérés de type “multi-chaîne” a été introduit dans [87]. Plusieurs stages ont permis l’implémentation partielle en Scilab, C ou C++, et le test de ce type d’algorithmes (voir le travail de Vishesh Dhingra [100]), ou de son couplage avec la résolution de systèmes linéaires par des méthodes multigrilles algébriques (stage de Shantanu Gangal en 2007). Le travail de thèse de Sylvie Detournay, qui porte sur le couplage entre itérations sur les politiques et méthodes multigrilles algébriques, voir le §6.4.1 ci-dessous, a permis le développement d’un programme complet. Le code écrit par Sylvie Detournay (en C) a été déposé sur InriaGForge. Pour le moment il n’est accessible qu’aux membres de l’équipe.

English version

The policy iteration algorithm for zero sum repeated games with ergodic payoff (i.e. mean payoff per time unit), and in degenerate “multichain” cases, has been introduced in [87]. Several internships allowed us to implement in Scilab, C or C++, and to test such algorithms (see the work of Vishesh Dhingra [100]), or its combinaison with the resolution of linear systems by algebraic multigrid methods (internship of Shantanu Gangal in 2007). The PhD thesis work of Sylvie Detournay, who concerns the combinaison of policy iterations with algebraic multigrid methods, see §6.4.1 below, allowed us to develop a complete program. The program written by Sylvie Detournay (in C language) has been posted on InriaGForge. For the moment it can only be seen by members of the team.
5.3. TPLib: bibliothèque pour la manipulation de polyèdres tropicaux/TPLib: tropical polyhedra library

TPLib est une bibliothèque écrite en OCaml qui permet de manipuler des polyèdres tropicaux. Elle est distribuée sous licence LGPL https://gforge.inria.fr/projects/tplib.

Cette bibliothèque implémente notamment des algorithmes permettant de passer d’une représentation externe d’un polyèdre à une représentation interne, ou inversement (voir §6.2.1 pour plus de détails). Elle permet aussi de réaliser d’autres opérations fondamentales, comme le calcul du complexe polyédral associé à un polyèdre donné (au sens de Develin et Sturmfels [98]), ou le calcul de cônes tangents tropicaux. Enfin, elle fournit toutes les primitives permettant d’utiliser les polyèdres tropicaux en tant que domaine abstrait numérique, afin de déterminer des invariants de programmes ou systèmes faisant intervenir les opérations $\min$ et $\max$ (voir [67]).

TPLib est aujourd’hui utilisé dans le logiciel Polymake [117], développé à la Technische Universität Darmstadt (Allemagne). Ce dernier logiciel constitue une boîte à outils permettant de manipuler des nombreux objets mathématiques (polytopes convexes, complexes polyédraux, graphes, matroïdes, polytopes tropicaux).

Le développement d’interfaces avec d’autres logiciels est désormais facilité grâce à la présence de bindings dans le langage C. Grâce à cela, un prototype d’interface a été réalisé entre TPLib et l’outil VerifyTAPN (https://launchpad.net/verifytapn), qui permet la vérification de réseaux de Pétri avec arcs temporisés (voir §6.5.7). De même, une interface à la bibliothèque de domaines abstraits numériques APRON [127] est également en cours de développement.

English version

TPLib is a library written in OCaml, which allows to manipulate tropical polyhedra. It is distributed under LGPL https://gforge.inria.fr/projects/tplib.

This library implements algorithms allowing to pass from an external representation of a polyhedron to an internal description, or inversely (see §6.2.1 for more details). Besides, the library allows to perform several fundamental operations over tropical polyhedra, such as computing the associated polyhedral complex (see Develin and Sturmfels [98]), or determining the tropical tangent cone at any point. Finally, it provides all the primitives allowing to use tropical polyhedra as an numerical abstract domain, in order to determine program/system invariants involving the operations $\min$ and $\max$ (see [67]).

TPLib is now used in the software Polymake [117], developed in Technische Universität Darmstadt (Germany). Polymake is a toolbox allowing to manipulate mathematical objects such as convex polytopes, polyhedral complexes, graphs, matroids, and tropical polytopes.

The development of further interfaces is now easier thanks to the distribution of bindings in C language. Using these bindings, a prototype of interface has been created between TPLib and the model-checker VerifyTAPN (https://launchpad.net/verifytapn), which allows the verification of timed-arc Petri Nets (see §6.5.7). An interface to the numerical abstract domain APRON [127] is also under development.
MCTAO Team (section vide)
5. Software

5.1. ORCCAD

Participants: Daniel Simon [correspondant], Soraya Arias [SED], Roger Pissard-Gibollet [SED].

ORCCAD is a software environment that allows for the design and implementation of the continuous and discrete time components of complex control systems, e.g. robotics systems which provided it first ground [59]. It also allows the specification and validation of complex missions to be performed by the system. It is mainly intended for critical real-time applications, in which automatic control aspects (servo loops) have to interact narrowly with the handling of discrete events (exception handling, mode switching). ORCCAD offers a complete and coherent vertical solution, ranging from the high level specification to real-time code generation. The ORCCAD V3 software was designed with proprietary tools that moreover are now becoming obsolete. ORCCAD V4 is currently deeply re-engineered to be compliant with open-source and free software tools (Java/Eclipse). Current targets are Linux (Posix threads) and Xenomai, a real-time development framework cooperating with the Linux kernel (http://www.xenomai.org). ORCCAD is supported by the Support Expérimentations & Développement (SED) service of INRIA-Rhône-Alpes. ORCCAD is used by the experimental robotics platforms of INRIA-Rhône-Alpes and by the Safenecs ANR project in a real-time simulator of a X4 drone. New functionalities and updates are developed jointly by the SED service and researchers of the NECS team. Web page: http://orccad.gforge.inria.fr.

5.2. MASim

Participants: J. Dumon [contact person], P. Bellemain [GIPSA-Lab], S. Nicolas [PROLEXIA], N. Maciol [PROLEXIA], F. Martinez [ROBOSOFT], J. Caquas [ROBOSOFT].

MASIM is a tool that has been adapted from our former multiagent simulator MUSim (MUSim=MASim + ConnectSim + ConnectIHM). It integrates agent's models, communication media including their limitations, heterogeneous network, and all the variants of the multi-agent control strategies. Besides the models and simulation engine, the simulation can be replayed through a GUI, an interactive graphical interface which is used to visualise and interpret the state of the multi-agent control system and communication topology. The validation scenario is a real-size application enough complex to enforce the pertinence of our results. The simulator MASim is now being used as an open research tool for various applications in the field of multi-agents networked systems, particularly within the FeedNetBack project (see Fig. 4).


5.3. GTL

Participants: C. Canudas de Wit [contact person], I. Bellicot [contact person], L. Leon Ojeda, D. Pisarski.

The team has created a software demonstrator to have a showcase including cutting-edge model developments. This software is a global services platform for end-user traffic use, providing accurate density calculation on traffic color vision, and integration of estimator and prediction motor for travel-time calculation. GTL (Grenoble Traffic Lab) is a real-time traffic data center platform intended to collect traffic road infrastructure information in real-time with minimum latency and fast sampling periods. The main elements of the GTL are: a real-time database, a show room, and a suit of traffic forecasting software. Sensed informations come from a dense wireless sensor network providing macroscopic traffic signals such as flows, velocities, densities, and magnetic signatures. This sensor network was set in place in collaboration with Inria spin-off Karrus-ITS, local traffic authorities (DIR-CE, CG38, La Metro), and specialized traffic research centers.
Figure 4. A scenario’s view obtained with MASIM.

Figure 5. The GTL Macro-simulator.
NON-A Project-Team (section vide)
CLASSIC Project-Team (section vide)
5. Software

5.1. ParadisEO

Participants: Clive Canape, Laetitia Jourdan, Arnaud Liefooghe, Nouredine Melab, Alexandre Quemy, El-Ghazali Talbi [correspondent], Sébastien Verel.

ParadisEO (PARallel and DIStributed Evolving Objects) is a C++ white-box object-oriented framework dedicated to the flexible design of metaheuristics. See web site http://paradiseo.gforge.inria.fr. Based on EO, a template-based ANSI-C++ compliant evolutionary computation library, it is composed of five modules:

- ParadisEO-EO provides tools for the development of population-based metaheuristics (evolutionary and genetic algorithm, genetic programming, particle swarm optimization, etc.)
- ParadisEO-MO provides tools for the development of single solution-based metaheuristics (hill-climbing, tabu search, simulated annealing, iterated local search, variable neighborhood search, incremental evaluation, partial neighborhood, etc.)
- ParadisEO-MOEO provides tools for the design of multi-objective metaheuristics (MO fitness assignment, MO diversity preservation, elitism, performance indicators, easy-to-use state-of-the-art algorithms, etc)
- ParadisEO-PEO provides tools for the design of parallel and distributed metaheuristics (parallel evaluation, parallel evaluation function, island model)
- ParadisEO-SMP provides tools for the design of shared memory parallel metaheuristics (parallel evaluation, island model)

Furthermore, ParadisEO also introduces tools for the design of distributed, hybrid and cooperative models:

- High level hybrid metaheuristics: coevolutionary and relay models.
- Low level hybrid metaheuristics: coevolutionary and relay models.

The ParadisEO framework has been especially designed to best suit to the following objectives:

- Maximum design and code reuse: ParadisEO is based on a clear conceptual separation of the solution methods from the problems they are intended to solve. This separation confers to the user a maximum code and design reuse.
- Flexibility and adaptability: The fine-grained nature of the classes provided by the framework allows a higher flexibility compared to other frameworks.
- Utility: ParadisEO allows the user to cover a broad range of metaheuristics, problems, parallel distributed models, hybridization mechanisms, etc.
- Transparent and easy access to performance and robustness: As the optimization applications are often time-consuming the performance issue is crucial. Parallelism and distribution are two important ways to achieve high performance execution. ParadisEO is one of the rare frameworks that provide the most common parallel and distributed models. These models can be exploited in a transparent way, one has just to instantiate their associated provided classes.
- Portability: The implemented models are portable on distributed-memory machines as well as on shared-memory multiprocessors, as they use standard libraries such as MPI and std::threads. ParadisEO supports the most recent version of standard of the C++ programming, c++11.

This year a new module, ParadisEO-SMP, has been released. All the new features is managed via the Inria Gforge project http://paradiseo.gforge.inria.fr. The version 2.0 has been released in Septembre 2012.
5.1.1. Paradiseo-SMP: a new module for shared memory parallel

This year, we released a new module dedicated to shared memory parallel. This module improves the technical mechanisms of Paradiseo-PEO thanks a new software architecture and the new c++11 features. Paradiseo-SMP implements parallel evaluation, dynamic heterogeneous island model, and their hybridization. The main features are:

- Dynamic Island Model: topology can be changed during the execution.
- Heterogeneous Islands: different kinds of population-based metaheuristics can communicate (evolutionary and genetic algorithm, particle swarm optimization, etc.).
- Island Model and master/slave model can be hybridized.

All these new features are developed in c++11.

5.1.2. New technical features

Regarding the technical aspects, the compatibility with dependencies taken into account is:

- c++11 features supporting.
- Checked compatibility with different operating systems.
- Reviewed and checked compatibility with new versions of the tools used (CMake, g++, clang, MinGW...).
- Unit and integration test of all additional components, and experiments on classical applications.

5.1.3. Contributions and documentations

Many investigations were made in this context in order to help users to manipulate the framework.

- New quick start guide is available.
- New tutorials:
  - Tutorials SMP.
  - Tutorials GPU.
- Updated implementation for classical problems.

Self-assessment of the team effort (software criteria: http://www.inria.fr/institut/organisation/instances/commission-d-evaluation)

(A-4-up5) Audience: 4 - Used in many universities for teaching and several companies.
(SO-4) Software Originality: 4 - ParadisEO aggregates the last results of the Dolphin team.
(SM-4) Software Maturity: 4 - Extensive documentation, strong software engineering and testing, regression testing, user feedback ...
(EM-2-up3) Evolution and Maintenance: 2 - Basic maintenance with persistent attention to users.
(SDL-4) Software Distribution and Licensing: 4 - CeCILL license, public source, Windows and Mac installer, Linux packages.
(OC) Own Contribution: (Design/Architecture) DA-4, (Coding/Debugging) CD-4, (Maintenance/Support) MS-4, (Team/Project Management) TPM-4
5. Software

5.1. FluidExponents

Participants: Denis Arrivault [correspondant], Hussein Yahia, Joel Sudre.

Denis Arrivault has joined the team for a complete refoundation, rewriting, generalization and diffusion of the FluidExponents software. FluidExponents is a software implementation of the MMF, presently written in Java, in a cooperative development mode on the Inria GForge, deposited at APP in 2010. The new software is presently in the phase of specification, and will be rewritten in C++, using existing libraries for data containers, mathematical computation and user interface. Denis Arrivault is recruited for a 24 month period on FluidExponents ADT.

During the new development, researchers still make use of the current version of the FluidExponents software written in Java, version number 0.8. Contact: denis.arrivault@inria.fr.
MISTIS Project-Team

5. Software

5.1. The ECMPR software

Participant: Florence Forbes.

Joint work with: Radu Horaud and Manuel Iguel.

The ECMPR (Expectation Conditional Maximization for Point Registration) package implements [57][65]. It registers two (2D or 3D) point clouds using an algorithm based on maximum likelihood with hidden variables. The method can register both rigid and articulated shapes. It estimates both the rigid or the kinematic transformation between the two shapes as well as the parameters (covariances) associated with the underlying Gaussian mixture model. It has been registered in APP in 2010 under the GPL license.

5.2. The LOCUS and P-LOCUS software

Participants: Florence Forbes, Senan James Doyle.

Joint work with: Michel Dojat.

From brain MR images, neuroradiologists are able to delineate tissues such as grey matter and structures such as Thalamus and damaged regions. This delineation is a common task for an expert but unsupervised segmentation is difficult due to a number of artefacts. The LOCUS software and its recent extension P-LOCUS automatically perform this segmentation for healthy and pathological brains. An image is divided into cubes on each of which a statistical model is applied. This provides a number of local treatments that are then integrated to ensure consistency at a global level, resulting in low sensitivity to artifacts. The statistical model is based on a Markovian approach that enables to capture the relations between tissues and structures, to integrate a priori anatomical knowledge and to handle local estimations and spatial correlations.

The LOCUS software has been developed in the context of a collaboration between Mistis, a computer science team (Magma, LIG) and a Neuroscience methodological team (the Neuroimaging team from Grenoble Institut of Neurosciences, INSERM). This collaboration resulted over the period 2006-2008 into the PhD thesis of B. Scherrer (advised by C. Garbay and M. Dojat) and in a number of publications. In particular, B. Scherrer received a “Young Investigator Award” at the 2008 MICCAI conference. Its extension (P-LOCUS) for lesion detection is realized by S. Doyle with financial support from Gravit for possible industrial transfer.

The originality of this work comes from the successful combination of the teams respective strengths i.e. expertise in distributed computing, in neuroimaging data processing and in statistical methods.

5.3. The POPEYE software

Participant: Florence Forbes.

Joint work with: Vasil Khalidov, Radu Horaud, Miles Hansard, Ramya Narasimha, Elise Arnaud.

POPEYE contains software modules and libraries jointly developed by three partners within the POP STREP project: Inria, University of Sheffield, and University of Coimbra. It includes kinematic and dynamic control of the robot head, stereo calibration, camera-microphone calibration, auditory and image processing, stereo matching, binaural localization, audio-visual speaker localization. Currently, this software package is not distributed outside POP.

5.4. The HDDA and HDCC toolboxes

Participant: Stéphane Girard.
Joint work with: Charles Bouveyron (Université Paris 1). The High-Dimensional Discriminant Analysis (HDDA) and the High-Dimensional Data Clustering (HDDC) toolboxes contain respectively efficient supervised and unsupervised classifiers for high-dimensional data. These classifiers are based on Gaussian models adapted for high-dimensional data [53]. The HDDA and HDDC toolboxes are available for Matlab and are included into the software MixMod [52]. Recently, a R package has been developed and integrated in The Comprehensive R Archive Network (CRAN). It can be downloaded at the following URL: http://cran.r-project.org/web/packages/HDclassif/.

5.5. The Extremes freeware

Participant: Stéphane Girard.

Joint work with: Diebolt, J. (CNRS), Laurent Gardes (Univ Strasbourg) and Garrido, M. (INRA Clermont-Ferrand-Theix).

The EXTREMES software is a toolbox dedicated to the modelling of extremal events offering extreme quantile estimation procedures and model selection methods. This software results from a collaboration with EDF R&D. It is also a consequence of the PhD thesis work of Myriam Garrido [55]. The software is written in C++ with a Matlab graphical interface. It is now available both on Windows and Linux environments. It can be downloaded at the following URL: http://extremes.gforge.inria.fr/.

5.6. The SpaCEM³ program

Participants: Senan James Doyle, Florence Forbes.

SpaCEM³ (Spatial Clustering with EM and Markov Models) is a software that provides a wide range of supervised or unsupervised clustering algorithms. The main originality of the proposed algorithms is that clustered objects do not need to be assumed independent and can be associated with very high-dimensional measurements. Typical examples include image segmentation where the objects are the pixels on a regular grid and depend on neighbouring pixels on this grid. More generally, the software provides algorithms to cluster multimodal data with an underlying dependence structure accounting for some spatial localisation or some kind of interaction that can be encoded in a graph.

This software, developed by present and past members of the team, is the result of several research developments on the subject. The current version 2.09 of the software is CeCILLB licensed.

Main features. The approach is based on the EM algorithm for clustering and on Markov Random Fields (MRF) to account for dependencies. In addition to standard clustering tools based on independent Gaussian mixture models, SpaCEM³ features include:

- The unsupervised clustering of dependent objects. Their dependencies are encoded via a graph not necessarily regular and data sets are modelled via Markov random fields and mixture models (eg. MRF and Hidden MRF). Available Markov models include extensions of the Potts model with the possibility to define more general interaction models.
- The supervised clustering of dependent objects when standard Hidden MRF (HMRF) assumptions do not hold (ie. in the case of non-correlated and non-unimodal noise models). The learning and test steps are based on recently introduced Triplet Markov models.
- Selection model criteria (BIC, ICL and their mean-field approximations) that select the "best" HMRF according to the data.
- The possibility of producing simulated data from:
  - general pairwise MRF with singleton and pair potentials (typically Potts models and extensions)
  - standard HMRF, ie. with independent noise model
  - general Triplet Markov models with interaction up to order 2
- A specific setting to account for high-dimensional observations.
- An integrated framework to deal with missing observations, under Missing At Random (MAR) hypothesis, with prior imputation (KNN, mean, etc), online imputation (as a step in the algorithm), or without imputation.
The software is available at http://spacem3.gforge.inria.fr. A user manual in English is available on the website above together with example data sets. The INRA Toulouse unit is more recently participating in this project for promotion among the bioinformatics community [75].

5.7. The FASTRUCT software

**Participant:** Florence Forbes.

**Joint work with:** Francois, O. (TimB, TIMC) and Chen, C. (former Post-doctoral fellow in Mistis).

The FASTRUCT program is dedicated to the modelling and inference of population structure from genetic data. Bayesian model-based clustering programs have gained increased popularity in studies of population structure since the publication of the software STRUCTURE [70]. These programs are generally acknowledged as performing well, but their running-time may be prohibitive. FASTRUCT is a non-Bayesian implementation of the classical model with no-admixture uncorrelated allele frequencies. This new program relies on the Expectation-Maximization principle, and produces assignment rivaling other model-based clustering programs. In addition, it can be several-fold faster than Bayesian implementations. The software consists of a command-line engine, which is suitable for batch-analysis of data, and a MS Windows graphical interface, which is convenient for exploring data.

It is written for Windows OS and contains a detailed user’s guide. It is available at http://mistis.inrialpes.fr/realisations.html.

The functionalities are further described in the related publication:

- Molecular Ecology Notes 2006 [56].

5.8. The TESS software

**Participant:** Florence Forbes.

**Joint work with:** Francois, O. (TimB, TIMC) and Chen, C. (former post-doctoral fellow in Mistis).

TESS is a computer program that implements a Bayesian clustering algorithm for spatial population genetics. Is it particularly useful for seeking genetic barriers or genetic discontinuities in continuous populations. The method is based on a hierarchical mixture model where the prior distribution on cluster labels is defined as a Hidden Markov Random Field [60]. Given individual geographical locations, the program seeks population structure from multilocus genotypes without assuming predefined populations. TESS takes input data files in a format compatible to existing non-spatial Bayesian algorithms (e.g. STRUCTURE). It returns graphical displays of cluster membership probabilities and geographical cluster assignments through its Graphical User Interface.

The functionalities and the comparison with three other Bayesian Clustering programs are specified in the following publication:

- Molecular Ecology Notes 2007
5. Software

5.1. Two advances for the MIXMOD software

Participants: Christophe Biernacki, Serge Iovleff, Remi Lebret, Parmeet Bhatia.

MIXMOD (MIXture MODelling) is an important software for the mΘdal team since it concerns its main topics: model-based supervised, unsupervised and semisupervised classification for various data situations. MIXMOD is now a well-distributed software with over 250 downloads/month are recorded for several years. MIXMOD is written in C++ (more than 10 000 lines) and distributed under GNU General Public License. Several other institutions participate in the MIXMOD development since several years: CNRS, Inria Saclay-Île de France, Université de Franche-Comté, Université Lille 1. The software already benefits from several APP deposits.

An interface between MIXMOD and R (Rmixmod) has been developed by Rémi Lebret and Serge Iovleff and is now available on the CRAN (http://cran.r-project.org/web/packages/Rmixmod/index.html). We expect now a wide impact of MIXMOD on the growing community familiar with R. A paper related to Rmixmod is submitted to an international journal [34].

Until December 2012, Parmeet Bhatia, under scientific supervision of Christophe Biernacki, is developing possibility in MIXMOD to cluster simultaneously continuous and categorical data with the restrictive conditional independence assumption. It is an important first step towards the long term purpose of mΘdal to cluster heterogeneous (or mixed) data sets.

5.2. The blockcluster package

Participants: Christophe Biernacki, Serge Iovleff, Parmeet Bhatia.

blockcluster is a R package for model-based simultaneous clustering of rows and columns, thanks to an Inria ADT grant (Parmeet Bhatia). It is also developed in collaboration with University of Technology of Compiègne. It offers the ability to structure very large data tables both in lines and columns for different data types (continuous, binary and contingency data). In particular, it opens wide potential applications in biology, marketing, etc. It is available online on CRAN (http://cran.r-project.org/web/packages/blockcluster/index.html) for all major platforms (Linux, MacOS, Windows). It also comes with utility functions to visualize data. A paper related to blockcluster is submitted to an international journal [40].

5.3. Cuvelust package

Participant: Guillemette Marot.

cuvelust is a R package dedicated to model-based curve clustering. Considered models include Functional Clustering Mixed Models (FCMM, ie functional clustering with the presence of functional random effects), but also traditional functional clustering model (FCM, without functional random effects), and functional mixed models (FMM, functional random effects without clustering). Estimation is done by maximum likelihood using the EM algorithm, and two criteria are proposed to select the number of clusters, based on integrated likelihoods.

Guillemette Marot was the main contributor of the beta version of the package during her post-doc. Due to several changes in conception and due to planning of extensions in the package by the other contributors of the package, she decided to become a regular contributor and left the maintenance to Franck Picard.

5.4. MetaMa

Participant: Guillemette Marot.
metaMA is a specialised software for microarrays. It is a R package which combines either p-values or modified effect sizes from different studies to find differentially expressed genes. The main competitor of metaMA is geneMeta. Compared to geneMeta, metaMA offers an improvement for small sample size datasets since the corresponding modelling is based on shrinkage approaches.

Guillemette Marot is the main contributor and the maintainer of these packages and spent around one year full time for this package between the conception, the implementation, and the documentation. Her PhD advisors (Florence Jaffrézic, Claus-Dieter Mayer, Jean-Louis Foulley) helped her with the conception but she implemented alone the code.

First versions were posted to the CRAN, the official website of the R software, in 2009. New versions for this package were released in August 2011 in order to take into account remarks from the main users (biologists or biostatisticians analysing gene expression data). This software is routinely used by biologists from INRA, Jouy en Josas (it has been included in a local analysis pipeline) but its diffusion on the CRAN makes it available to a wider community, as attested by the citations of publications related to the methods implemented in the software.

More information is available on the website [http://cran.r-project.org/web/packages/metaMA/](http://cran.r-project.org/web/packages/metaMA/)

### 5.5. SMVar
**Participant:** Guillemette Marot.

SMVar is a specialised software for microarrays. This R package implements the structural model for variances in order to detect differentially expressed genes from gene expression data. It performs gene expression differential analysis, based on a particular variance modelling. Its main competitor is the Bioconductor R package limma but limma assumes a common variance between the two groups to be compared while SMVar relaxes this assumption.

More information on the website [http://cran.r-project.org/web/packages/SMVar/index.html](http://cran.r-project.org/web/packages/SMVar/index.html)

### 5.6. Tax3 Software
**Participants:** Serge Iovleff, Remi Lebret.

Tax3 implements a statistical method providing an analytical framework for high dimensional datasets and complex problems combining several variable types: genetics, genomics, biomarkers and phenotypes.

### 5.7. aam Program
**Participant:** Serge Iovleff.

aam is a console based program dedicated to the estimation of the semi-linear auto-associative models in a gaussian setting. It is written in C++ and used the STK++ library as support.

### 5.8. STK++
**Participant:** Serge Iovleff.

STK++ is a multi-platform toolkit written in C++ for creating fast and easy to use data mining programs. It offers a large set of templated class in C++ which are suitable for projects ranging from small one-off projects to complete statistical application suites. A C equivalent would be gsl. However, STK++ is developed in C++ in order to get speed and reusability.

As the aim of STK++ is to aid developers to new developments, it proposes essentially interfaces classes and various concrete helping classes, like arrays, numerical methods (QR, SVD), input and output (csv files), random number generators, etc.
The software is regularly developed for 10 years by Serge Iovleff and it is a work in progress. The version 0.3 has been released. More information is available on the website http://www.stkpp.org/ and source repository is here: https://sourcesup.cru.fr/projects/stk/

5.9. Scan3D

Participants: Alexandru Amarioarei, Cristian Preda.

Scan3D is a C++ software for estimating the distribution of the three-dimensional scan statistics for Bernoulli and Poisson models. It implements the most recent approximation methods available, in particular that developed by the authors providing bounds for the approximation errors [39].
5. Software

5.1. BaPCod – a generic Branch-and-Price Code

Participants: Romain Leguay [Software Engineer], Pierre Pesneau, Ruslan Sadykov, François Vanderbeck [correspondant].

BaPCod is a prototype code that solves Mixed Integer Programs (MIP) by application of a Dantzig-Wolfe reformulation technique. The reformulated problem is solved using a branch-and-price (column generation) algorithm. This software platform, made of C++ classes, offers a “black-box” implementation that does not require user input and is not application specific. The features are

(i) the automation of the Dantzig-Wolfe reformulation process (the user defines a mixed integer programming problem in a pseudo modeling language, defining variables and constraints, identifying subproblems. He can provide subproblem solvers if available, but he does not need to explicitly define the reformulation, the explicit form of the columns, their reduced cost, or the Lagrangian bounds.

(ii) a default column generation procedure with standard initialization and stabilization [1], [23] [25] [29] [32] and

(iii) a default branching scheme that is generic to all applications [9],

(iv) default primal heuristics specially developed for use in a decomposition framework [49], [27], [30].

The prototype software was/is used as background solver for 5 PhD thesis. It also served as the framework for our comparative study in a Inria collaborative research action [1]. It has been experimented by two of our industrial partners, Exeo Solutions (Bayonne), on an inventory routing problem, and Orange Lab (France Telecom, Paris) on network design problems. The prototype also enables us to be very responsive in our industrial contact.

See also the web page https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod.
5. Software

5.1. MIXMOD software

Participants: Gilles Celeux [Correspondant], Erwan Le Pennec.

Mixture model, cluster analysis, discriminant analysis

MIXMOD is being developed in collaboration with Christophe Biernacki, Florent Langrognet (Université de Franche-Comté) and Gérard Govaert (Université de Technologie de Compiègne). MIXMOD (MIXture MODelling) software fits mixture models to a given data set with either a clustering or a discriminant analysis purpose. MIXMOD uses a large variety of algorithms to estimate mixture parameters, e.g., EM, Classification EM, and Stochastic EM. They can be combined to create different strategies that lead to a sensible maximum of the likelihood (or completed likelihood) function. Moreover, different information criteria for choosing a parsimonious model, e.g., the number of mixture component, some of them favoring either a cluster analysis or a discriminant analysis viewpoint, are included. Many Gaussian models for continuous variables and multinomial models for discrete variable are available. Written in C++, MIXMOD is interfaced with SCILAB and MATLAB. The software, the statistical documentation and also the user guide are available on the Internet at the following address: http://www.mixmod.org.

Since this 2010, MIXMOD has a proper graphical user interface (Version 1) which has been presented at the MIXMOD day in Lyon in December 2010. A version of MIXMOD in R is now available http://cran.r-project.org/web/packages/Rmixmod/index.html.

Erwan Le Pennec with the help of Serge Cohen has proposed a spatial extension in which the mixture weights can vary spatially.
5. Software

5.1. Introduction

In 2012, SEQUEL continued the development of software for computer games (notably Go) and also developed two novel libraries for functional regression and data mining.

5.2. Computer Games

Participant: Rémi Coulom.

We continued the development of three main softwares for computer games:

- **Crazy Stone** is a top-level Go-playing program that has been developed by Rémi Coulom since 2005. Crazy Stone won several major international Go tournaments in the past. In 2012, a new version was released in Japan. This new version won a game with a 4-stone handicap against a professional player during the European Go Congress in Bonn, Germany. It is distributed as a commercial product by Unbalance Corporation (Japan). 6-month work in 2012. URL: [http://remi.coulom.free.fr/CrazyStone/](http://remi.coulom.free.fr/CrazyStone/)

- **Crazy Hanafuda** is a program to play the Japanese card game of Hanafuda. One month of work in 2012. A licence agreement was signed with Unbalance Corporation in January. The Windows 8 version of the program was released commercially in November.


5.3. Vowpal Wabbit

Participants: Jérémie Mary, Romaric Gaudel, Thomas Chabin.

Vowpal Wabbit is a GPL project leaded by John Langford at Yahoo! Research and now at Microsoft. The goal is to build a very fast, distributed and large scale machine learning software. [https://github.com/JohnLangford/vowpal_wabbit/wiki](https://github.com/JohnLangford/vowpal_wabbit/wiki). We worked on the optimization of the parser and on the memory structures of the i/o. The modifications have been accepted for commit in the main branch and allow an average division by two of all execution times.
5. Software

5.1. SPAMS (SPArse Modeling Software)

**Participants:** Jean-Paul Chieze [correspondant], Guillaume Obozinski [correspondant].

SPAMS (SPArse Modeling Software) is an optimization toolbox for solving various sparse estimation problems: dictionary learning and matrix factorization, solving sparse decomposition problems, solving structured sparse decomposition problems. It is developed by Julien Mairal (former Willow PhD student, co-advised by F. Bach and J. Ponce), with the collaboration of Francis Bach (Inria), Jean Ponce (Ecole Normale Superieure), Guillermo Sapiro (University of Minnesota), Rodolphe Jenatton (Inria) and Guillaume Obozinski (Inria). It is coded in C++ with a Matlab interface. Recently, interfaces for R and Python have been developed by Jean-Paul Chieze (Inria). Currently 650 downloads and between 1500 and 2000 page visits per month. See http://spams-devel.gforge.inria.fr/.

5.2. SiGMa - Simple Greedy Matching: a tool for aligning large knowledge-bases

**Participant:** Simon Lacoste-Julien [correspondant].

SiGMa - Simple Greedy Matching: a tool for aligning large knowledge-bases


The tool SiGMa (Simple Greedy Matching) is a knowledge base alignment tool implemented in Python. It takes as input two knowledge bases, each represented as a list of triples of (entity, relationship, entity), in addition to a partial alignment between the relationships from one knowledge base to the other, and gives as output an ordered list of proposed entity matches between the two knowledge base (where the order corresponds heuristically to a notion of certainty about these matches). The matching decisions are made in a greedy fashion, combining information about the relationship graph as well as a pairwise similarity scores defined between the entities. The code handles various sources of information to be used for this score, such as a similarity defined on strings, dates, and other entity properties – and gives a few options to the user.

We also provide two large-scale knowledge base alignment benchmark datasets with tens of thousands of ground truth pairs: YAGO aligned to IMDb as well as Freebase aligned to IMDb.

Participants outside of Sierra: Konstantina Palla, Alex Davies, Zoubin Ghahramani (Machine Learning Group, Department of Engineering, University of Cambridge); Gjergji Kasneci, Thore Graepel (Microsoft Research Cambridge)

See http://mlg.eng.cam.ac.uk/slacoste/sigma/.

5.3. minFunc (2012 version)

**Participant:** Mark Schmidt [correspondant].

minFunc is a Matlab function for unconstrained optimization of differentiable real-valued multivariate functions using line-search methods. It uses an interface very similar to the Matlab Optimization Toolbox function fminunc, and can be called as a replacement for this function. On many problems, minFunc requires fewer function evaluations to converge than fminunc (or minimize.m). Further it can optimize problems with a much larger number of variables (fminunc is restricted to several thousand variables), and uses a line search that is robust to several common function pathologies.
The default parameters of minFunc call a quasi-Newton strategy, where limited-memory BFGS updates with Shanno-Phua scaling are used in computing the step direction, and a bracketing line-search for a point satisfying the strong Wolfe conditions is used to compute the step direction. In the line search, (safeguarded) cubic interpolation is used to generate trial values, and the method switches to an Armijo back-tracking line search on iterations where the objective function enters a region where the parameters do not produce a real valued output (i.e. complex, NaN, or Inf). See http://www.di.ens.fr/~mschmidt/Software/minFunc.html.

5.4. prettyPlot

Participant: Mark Schmidt [correspondant].

The prettyPlot function is a simple wrapper to Matlab’s plot function for quickly making nicer-looking plots. Here are the features: Made the default line styles bigger, and the default fonts nicer. Options are passed as a structure, instead of through plot’s large number of different functions. You can pass in cell arrays to have lines of different lengths. You can pass an \( n \times 3 \) matrix of colors, and cell arrays of line-styles and/or markers. It will cycle through the given choices. All markers are placed on top of (all) lines, you do not have to put a marker on every data point, and you can use different spacing between markers for different lines. You can change only the upper or lower x-limit (y-limit), rather than having to specify both. There is some support for making nicer-looking error lines. See http://www.di.ens.fr/~mschmidt/Software/prettyPlot.html.

5.5. SegAnnot

Participant: Toby Hocking [correspondant].

SegAnnot: an R package for fast segmentation of annotated piecewise constant signals. Tech report and R package. Standard segmentation models for piecewise constant signals do not always agree with an expert’s visual interpretation of the signal, as encoded using a set of annotations. This R package implements a dynamic programming algorithm which can be used to quickly find a segmentation model in agreement with expert annotations. Collaboration with Guillem Rigaill (Inria - AgroParisTech). See http://hal.inria.fr/hal-00759129 and http://segannot.r-forge.r-project.org/.
5. Software

5.1. Metis

Participants: Olivier Teytaud [correspondent], Adrien Couëtoux, Jérémie Decock, Jean-Joseph Christophe.

Energy, Optimization, Planning

Many works in Energy Optimization, in particular in the case of high-scale sequential decision making, are based on one software per application, because optimizing the software eventually implies losing generality. Our goal is to develop with Artelys a platform, Metis, which can be used for several applications. In 2012 we interfaced existing codes in Artelys and codes developed in the Tao team; experiments have been performed and test cases have been designed. A main further work is the introduction of generic tools for stochastic dynamic programming into the platform, for comparison and hybridization with other tools from the UCT-SIG.

Our favorite challenge is the hybridization of “classical” tools (based on constraint satisfaction problems, or mixed integer linear programming or mixed integer quadratic programming), which are fast and accurate, with non-linear solvers which can take care of a sophisticated (non-linear) model.

5.2. MoGo

Participants: Olivier Teytaud [correspondent], Hassen Doghmen, Jean-Baptiste Hoock.

Go, Multi-armed bandit

MoGo and its Franco-Taiwanese counterpart MoGoTW is a Monte-Carlo Tree Search program for the game of Go, which made several milestones of computer-Go in the past (first wins against professional players in 19x19; first win with disadvantageous side in 9x9 Go). Recent results include 7 wins out of 12 against professional players (in Brisbane, 2012). However, the work in the UCT-SIG has now shifted to energy management.

5.3. CMA-ES: Covariance Matrix Adaptation Evolution Strategy

Participant: Nikolaus Hansen [correspondent].

Evolutionary Computation, stochastic optimization, real-parameter optimization

The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is one of the most powerful continuous domain evolutionary algorithms. The CMA-ES is considered state-of-the-art in continuous domain evolutionary computation and has been shown to be highly competitive on different problem classes. The algorithm is widely used in research and industry as witnessed by hundreds of published applications. We provide source code for the CMA-ES in C, Java, Matlab, Octave, Python, and Scilab including the latest variants of the algorithm.

Links: http://www.lri.fr/~hansen/cmaes_inmatlab.html

5.4. COMparing Continuous Optimizers

Participants: Nikolaus Hansen [correspondent], Anne Auger, Marc Schoenauer.

Evolutionary Computation, stochastic optimization, real-parameter optimization, benchmarking, derivative free optimization

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COCO (COmparing Continuous Optimizers) is a platform for systematic and sound comparisons of real-parameter global optimizers. COCO provides benchmark function testbeds (noiseless and noisy) and tools for processing and visualizing data generated by one or several optimizers. The code for processing experiments is provided in Matlab and C. The post-processing code is provided in Python. The code is under continuous development and has been used for the GECCO 2009, 2010 and 2012 workshops on “Black Box Optimization Benchmarking” (BBOB) (see Section 3.3), and serves as a basis for the test platform in the CSDL project.

Link: http://coco.gforge.inria.fr/doku.php

5.5. MultiBoost

Participants: Balázs Kégl [correspondent], Djalel Benbouzid.

multi-class, multi-label classification

The MultiBoost package [4] provides a fast C++ implementation of multi-class/multi-label/multi-task boosting algorithms. It is based on AdaBoost.MH but it also implements popular cascade classifiers, Arc-GV, and FILTERBOOST. The package contains common multi-class base learners (stumps, trees, products, Haar filters). Further base learners and strong learners following the boosting paradigm can be easily implemented in a flexible framework.

Link: http://multiboost.org

5.6. Grid Observatory

Participants: Cécile Germain [correspondent], Julien Nauroy, Michèle Sebag.

Autonomic Computing, Green Computing The Grid Observatory software suite collects and publishes traces of the EGI (European Grid Initiative) grid usage. With the release and extensions of its portal, the Grid Observatory has made a database of grid usage traces available to the wider computer science community. These data are stored on the grid, and made accessible through a web portal without the need of grid credentials. More than 140 users are currently registered. The GO is supported by an Inria ADT (Action de Développement Technologique).

The Green Computing Observatory (GCO), part of the GO initiative monitors a large computing center (Laboratoire de l’Accélérateur Linéaire - LAL) within the EGI grid, and publishes the data through the Grid Observatory. A tool has been made available to provide interactive visualization of the site activity (load, power usage and more) at the global and individual level. The GCO is supported by the CNRS PEPS program, and by University Paris-Sud through the MRM (Moyens de Recherche Mutualisés) program. The first barrier to improved energy efficiency is the lack of overall data collection on the energy consumption of individual components of data centers. The Green Computing Observatory collects monitoring data on energy consumption of a large computing center, and publishes them through the Grid Observatory portal. These data include the detailed monitoring of the processors and motherboards, as well as global site information, such as overall consumption and external temperature, as global optimization is a promising way of research. A second barrier is making the collected data usable. The difficulty is to make the data readily consistent and complete, as well as understandable for further exploitation. For this purpose, the GCO opts for an ontological approach in order to rigorously define the semantics of the data (what is measured) and the context of their production (how are they acquired and/or calculated). The first achievements of these developments have been described in [40], and presented at the ICT-COST meeting and GreenDays@Lyon.

Link: http://grid-observatory.org
5. Software

5.1. BiiPS software

BiiPS is a general software, developed by Adrien Todeschini, for Bayesian inference with interacting particle systems, a.k.a. sequential Monte Carlo (SMC) methods. It aims at popularizing the use of these methods to non-statistician researchers and students, thanks to its automated “black box” inference engine.

It borrows from the BUGS/JAGS software, widely used in Bayesian statistics, the statistical modeling with graphical models and the language associated with their descriptions.

Unlike MCMC methods used by BUGS/JAGS, SMC methods are more adapted to dynamic problems (tracking, signal filtering, etc).

A beta version of the software can be downloaded from the website of the BiiPS project. This software has been presented at the international workshop BayesComp in Kyoto, the international conference ISBA in Tokyo, the conference on Premières Rencontres R in Bordeaux, and the international workshop on efficient simulation in finance in Paris.
ASPI Project-Team (section vide)
CQFD Project-Team  (section vide)
I4S Team

5. Software

5.1. COSMAD

With the help of former engineers, I4S team has developed and maintained a Scilab toolbox devoted to modal analysis and vibration monitoring of structures or machines subjected to known or ambient (unknown) excitation. This software (COSMAD 3.64) has been registered at the APP under the number

IDDN.FR.001.210011.002.S.A.2003.000.20700

A list of test-cases (simulators, laboratory test-beds, real structures) for which COSMAD has been used is available on I4S website. The problem is to identify the eigenstructure (eigenvalues and observed components of the associated eigenvectors) of the state transition matrix of a linear dynamical system, using only the observation of some measured outputs summarized into a sequence of covariance matrices corresponding to successive time shifts. Other services are

- Output-only and Input/Output subspace-based identification,
- Automated on-line identification package,
- Subspace-based identification through moving sensors data fusion,
- Damage detection and monitoring,
- Damage localization,

The modules have been tested by different partners, especially the French industrial partners, EADS, Dassault and Sopemea, within the FLITE2 project, by partners from the past CONSTRUCTIF project, and within the framework of bilateral contracts with SNECMA and SVS.

Based on intensive internal evaluation of the toolbox, on both simulated and real data sets, EADS Space Transportation and CNES have been investigating how to use the toolbox for the exploitation of the Ariane 5 flight data sets.

This Scilab toolbox continues to play the role of a programming and development environment for all our newly designed algorithms. Moreover, offering a maintained Scilab platform turns out to be a crucial factor in convincing industrial partners to undertake joint investigations with us. Just recently, SNECMA funded development for the Cosmad toolbox in 2010.

5.2. Prototypes

Three software have been deposed to the Agency of Program Protection, i.e.

- 1/ VIBRA-PARTICULAIRE : APP IDDN.FR.001.420016.000.S.P.2012.000.20700

They will be transferred to partners and industrial contracts when possible.

+ A new version of the COSMAD toolbox has been deposed at APP and concerns the transfer to SVS action.
4. Software

4.1. PREMIA

Participants: Antonino Zanette, Mathrisk Research team, Agnès Sulem [correspondant].

Premia is a software designed for option pricing, hedging and financial model calibration. It is provided with its C/C++ source code and an extensive scientific documentation. https://www-rocq.inria.fr/mathfi/Premia

The Premia project keeps track of the most recent advances in the field of computational finance in a well-documented way. It focuses on the implementation of numerical analysis techniques for both probabilistic and deterministic numerical methods. An important feature of the platform Premia is the detailed documentation which provides extended references in option pricing.

Premia is thus a powerful tool to assist Research & Development professional teams in their day-to-day duty. It is also a useful support for academics who wish to perform tests on new algorithms or pricing methods without starting from scratch.

Besides being a single entry point for accessible overviews and basic implementations of various numerical methods, the aim of the Premia project is:

1. to be a powerful testing platform for comparing different numerical methods between each other;
2. to build a link between professional financial teams and academic researchers;
3. to provide a useful teaching support for Master and PhD students in mathematical finance.

- AMS: 91B28;65Cxx;65Fxx;65Lxx;65Pxx
- License: Licence Propriétaire (genuin license for the Consortium Premia)
- Type of human computer interaction: Console, interface in Nsp, Web interface
- OS/Middelware: Linux, Mac OS X, Windows
- APP: The development of Premia started in 1999 and 14 are released up to now and registered at the APP agency.
- Programming language: C/C++ librairie Gtk
- Documentation: the PNL library is interfaced via doxygen
- Size of the software: 11 Mbyte of code split into 275,000 lines. 93 Mbyte of PDF files of documentation
- Publications: [1] [64] [78] [89] [95], [47]

4.1.1. Content of Premia

Premia contains various numerical algorithms (Finite-differences, trees and Monte-Carlo) for pricing vanilla and exotic options on equities, interest rate, credit and energy derivatives.

1. Equity derivatives:

The following models are considered:

- Black-Scholes model (up to dimension 10), stochastic volatility models (Hull-White, Heston, Fouque-Papanicolaou-Sircar), models with jumps (Merton, Kou, Tempered stable processes, Variance gamma, Normal inverse Gaussian), Bates model.

For high dimensional American options, Premia provides the most recent Monte-Carlo algorithms: Longstaff-Schwartz, Barraquand-Martineau, Tsitsklis-Van Roy, Broadie-Glassermann, quantization methods and Malliavin calculus based methods.

Dynamic Hedging for Black-Scholes and jump models is available.
Calibration algorithms for some models with jumps, local volatility and stochastic volatility are implemented.

2. **Interest rate derivatives**

The following models are considered:


Premia provides a calibration toolbox for Libor Market model using a database of swaptions and caps implied volatilities.

3. **Credit derivatives: CDS, CDO**

Reduced form models and copula models are considered.

Premia provides a toolbox for pricing CDOs using the most recent algorithms (Hull-White, Laurent-Gregory, El Karoui-Jiao, Yang-Zhang, Schönbucher)

4. **Hybrid products**

PDE solver for pricing derivatives on hybrid products like options on inflation and interest or change rates is implemented.

5. **Energy derivatives: swing options**

Mean reverting and jump models are considered.

Premia provides a toolbox for pricing swing options using finite differences, Monte-Carlo Malliavin-based approach and quantization algorithms.

### 4.1.2. Premia design

Anton Kolotaev (ADT engineer), supervised by J. Lelong, has developed a web platform allowing online tests ([https://quanto.inria.fr/premia/koPremia](https://quanto.inria.fr/premia/koPremia)). This online version allow us to supply benchmarks both for professional R&D teams and academics in mathematical finance. This will considerably increase the impact and the visibility of the software. Up to now, to use the opensource version of the software, one has to download from Premia’s website and install it on its own computer and this had become a brake on using Premia. Providing an online version of Premia is an original way of keeping up with the new standards of software usability without focusing too much on a dedicated solution per operation system.

To enable an advanced usage of Premia without being an advanced C or C++ programmer, we have started to implement Python bindings. The choice of Python has been quite obvious as Python has become over the past few years a standard cross–platform interpreted language for numerical problems.

Premia has managed to grow up over a period of more than a dozen years; this has been possible only because contributing an algorithm to Premia is subject to strict rules, which have become too stringent. To facilitate contributions, a standardized numerical library (PNL) has been developed under the LGPL since 2009, which offers a wide variety of high level numerical methods for dealing with linear algebra, numerical integration, optimization, random number generators, Fourier and Laplace transforms, and much more. Everyone who wishes to contribute is encouraged to base its code on PNL and providing such a unified numerical library has considerably eased the development of new algorithms which have become over the releases more and more sophisticated. An effort will be made to continue and stabilize the development of PNL.

### 4.1.3. Algorithms implemented in Premia in 2012

Premia 14 was delivered to the consortium members in March 2012. It contains the following new algorithms:

- **Interest Rate Derivatives**
  - An n-Dimensional Markov-functional Interest Rate Model
    - L. Kaisajuntti J. Kennedy. Preprint 2008
  - Efficient log-Levy approximations for Levy-driven Libor model.

- **Energy and Commodities**
  - Efficient pricing of Swing options in Lévy-driven models. O. Kudryavtsev, A. Zanette.

- **Credit Risk Derivatives**
  - Calibration in a local and stochastic intensity model. A. Alfonsi, C. Labart, J. LeLong

- **Equity Derivatives**
  - Forward Variance Dynamics: Bergomi’s model revisited. S.M. Ould Aly
  - Volatility of Volatility Expansion for Bergomi’s model. S.M. Ould Aly
  - A Mean-Reverting SDE on Correlation Matrices. A. Alfonsi, A. Ahdida
  - High order discretization schemes for stochastic volatility models. B. Jourdain, M. Sbai. *Quantitative Finance, to appear*
  - Wiener-Hopf techniques for Lookback options. O. Kudryavtsev
  - Analytical formulas for local volatility model with stochastic rates. E. Benhamou, E. Gobet, M. Miri 2009
  - American options in high dimension solving EDSR with penalization C. Labart, J. LeLong

The software Premia 14 has been deposited at the APP (Agence pour la Protection des Programmes) with the reference IDDN.FR.001.190010.011.S.C.2001.000.31000.
5. Software

5.1. FracLab

Participants: Paul Balança, Jacques Lévy Véhel [correspondant].

FracLab was developed for two main purposes:

1. propose a general platform allowing research teams to avoid the need to re-code basic and advanced techniques in the processing of signals based on (local) regularity.
2. provide state of the art algorithms allowing both to disseminate new methods in this area and to compare results on a common basis.

FracLab is a general purpose signal and image processing toolbox based on fractal, multifractal and local regularity methods. FracLab can be approached from two different perspectives:

- (multi-) fractal and local regularity analysis: A large number of procedures allow to compute various quantities associated with 1D or 2D signals, such as dimensions, Hölder and 2-microlocal exponents or multifractal spectra.
- Signal/Image processing: Alternatively, one can use FracLab directly to perform many basic tasks in signal processing, including estimation, detection, denoising, modeling, segmentation, classification, and synthesis.

A graphical interface makes FracLab easy to use and intuitive. In addition, various wavelet-related tools are available in FracLab.

FracLab is a free software. It mainly consists of routines developed in MatLab or C-code interfaced with MatLab. It runs under Linux, MacOS and Windows environments. In addition, a “stand-alone” version (i.e. which does not require MatLab to run) is available.

FracLab has been downloaded several thousands of times in the last years by users all around the world. A few dozen laboratories seem to use it regularly, with more than two hundreds registered users. Our ambition is to make it the standard in fractal softwares for signal and image processing applications. We have signs that this is starting to become the case. To date, its use has been acknowledged in more than two hundreds research papers in various areas such as astrophysics, chemical engineering, financial modeling, fluid dynamics, internet and road traffic analysis, image and signal processing, geophysics, biomedical applications, computer science, as well as in mathematical studies in analysis and statistics (see http://fraclab.saclay.inria.fr/ for a partial list with papers). In addition, we have opened the development of FracLab so that other teams worldwide may contribute. Additions have been made by groups in Australia, England, France, the USA, and Serbia.

We have produced this year a major release of FracLab (version 2.1).
5. Software

5.1. CarbonQuant

**Participant:** Mireille Bossy [correspondant].

CarbonQuant is a simulator project of CO2 allowances prices on a EU-ETS type market, by an indifference price approach.

It aims to demonstrate the high potentiality of stochastic control solvers, to quantify sensibilities of a carbon market with respect to its design.

Starting in September 2011, CarbonQuant is an ADT \(^1\) Inria.

See also the web page [http://carbonvalue.gforge.inria.fr](http://carbonvalue.gforge.inria.fr).

- Version: 0.1

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\(^1\) Technology Development Action