



RESEARCH CENTER

FIELD

**Applied Mathematics, Computation  
and Simulation**

# Activity Report 2017

## Section Software

Edition: 2018-02-19



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## ACUMES Project-Team

# 5. New Software and Platforms

## 5.1. MGDA

*Multiple Gradient Descent Algorithm*

KEYWORDS: Descent direction - Multiple gradients - Multi-objective differentiable optimization

SCIENTIFIC DESCRIPTION: The software provides a vector  $d$  whose scalar product with each of the given gradients (or directional derivative) is positive provided a solution exists. When the gradients are linearly independent, the algorithm is direct following a Gram-Schmidt orthogonalization. Otherwise, a sub-family of the gradients is identified according to a hierarchical criterion as a basis of the spanned subspace associated with a cone that contains almost all the gradient directions. Then, one solves a quadratic programming problem formulated in this basis.

<https://hal.inria.fr/hal-01139994> <https://hal.inria.fr/hal-01414741>

FUNCTIONAL DESCRIPTION: The utilization of the platform can be made via two modes : – the interactive mode, through a web interface that facilitates the data exchange between the user and an Inria dedicated machine, – the iterative mode, in which the user downloads the object library to be included in a personal optimization software.

- Participant: Jean-Antoine Désidéri
- Contact: Jean-Antoine Désidéri
- URL: <http://mgda.inria.fr>

## 5.2. Igloo

*Iso-Geometric anaLysis using discOntinuOus galerkin methods*

KEYWORDS: Numerical simulations - Isogeometric analysis

SCIENTIFIC DESCRIPTION: Igloo contains numerical methods to solve partial differential equations of hyperbolic type, or convection-dominant type, using an isogeometric formulation (NURBS bases) with a discontinuous Galerkin method.

FUNCTIONAL DESCRIPTION: Igloo is composed of a set of C++ libraries and applications, which allow to simulate time-dependent physical phenomena using natively CAD-based geometry descriptions.

- Author: Régis Duvigneau
- Contact: Régis Duvigneau

## 5.3. BuildingSmart

*BuildingSmart interactive visualization*

KEYWORDS: Physical simulation - 3D rendering - 3D interaction

SCIENTIFIC DESCRIPTION: The aim of the BuildingSmart project is to develop a software environment for the simulation and interactive visualisation for the design of buildings (structural safety, thermal confort).

FUNCTIONAL DESCRIPTION: The main task of the project is to study and develop solutions dedicated to interactive visualisation of building performances (heat, structural) in relation to the Building Information Modeling BIM framework, using Oculus Rift immersion.

NEWS OF THE YEAR: Demo movies are available from Youtube (see web site)

- Participants: Régis Duvigneau, Jean-Luc Szpyrka, David Rey and Clement Welsch
- Contact: Abderrahmane Habbal
- URL: [http://youtu.be/MW\\_gIF8hUdk](http://youtu.be/MW_gIF8hUdk)

## CAGIRE Project-Team

## 6. New Software and Platforms

### 6.1. AeroSol

**KEYWORD:** Finite element modelling

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

**NEWS OF THE YEAR:** The following points have been developed in the code

\*A postprocessing in the high order GMSH format has been added

\*On the Uhaina part, the work has been focused on the entropy viscosity approach for shock limiting, and on the positivity preserving limiters for ensuring positive water height

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

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

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

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

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

## CARDAMOM Project-Team

## 6. New Software and Platforms

### 6.1. AeroSol

**KEYWORD:** Finite element modelling

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

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

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

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

### 6.2. Crysa

**KEYWORDS:** Image analysis - 2D

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

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

### 6.3. Cut-ANOVA

*Cut-ANOVA Global Sensitivity Analysis*

**KEYWORDS:** Stochastic models - Uncertainty quantification

**SCIENTIFIC DESCRIPTION:** An anchored analysis of variance (ANOVA) method is proposed to decompose the statistical moments. Compared to the standard ANOVA with mutually orthogonal component functions, the anchored ANOVA, with an arbitrary choice of the anchor point, loses the orthogonality if employing the same measure. However, an advantage of the anchored ANOVA consists in the considerably reduced number of deterministic solver's computations, which renders the uncertainty quantification of real engineering problems much easier. Different from existing methods, the covariance decomposition of the output variance is used in this work to take account of the interactions between non-orthogonal components, yielding an exact variance expansion and thus, with a suitable numerical integration method, provides a strategy that converges. This convergence is verified by studying academic tests. In particular, the sensitivity problem of existing methods to the choice of anchor point is analyzed via the Ishigami case, and we point out that covariance decomposition survives from this issue. Also, with a truncated anchored ANOVA expansion, numerical results prove that the proposed approach is less sensitive to the anchor point. The covariance-based sensitivity indices (SI) are also used, compared to the variance-based SI. Furthermore, we emphasize that the covariance decomposition can be generalized in a straightforward way to decompose higher-order moments. For academic problems, results show the method converges to exact solution regarding both the skewness and kurtosis. The proposed method can indeed be applied to a large number of engineering problems.

**FUNCTIONAL DESCRIPTION:** The Cut-ANOVA code (Fortran 90, MPI + OpenMP) is devoted to the stochastic analysis of numerical simulations. The method implemented is based on the spectral expansion of "anchored ANOVA", allowing the covariance-based sensitivity analysis. Compared to the conventional Sobol method, "Cut-ANOVA" provides three sensitivity indices instead of one, which allows a better analysis of the reliability of the numerical prediction. On the other hand, "Cut-ANOVA" is able to compute the higher order statistical moments such as the Skewness (3-rd order moment) and Kurtosis (4-th order moment). Several dimension reduction techniques have also been implemented to reduce the computational cost. Finally, thanks to the innovative method implemented into the Code Cut-ANOVA, one can obtain a similar accuracy for stochastic quantities by using a considerably less number of deterministic model evaluations, compared with the classical Monte Carlo method.

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

## 6.4. Fmg

**KEYWORD:** Mesh adaptation

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

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

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

## 6.5. Mmg

*Mmg Platform*

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

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

The 3 softwares can be used by command line or using the library version (C, C++ and Fortran API) : - Mmg2d performs mesh generation and isotropic and anisotropic mesh adaptation. - Mmgs allows isotropic and anisotropic mesh adaptation for 3D surface meshes. - Mmg3d is a new version of the MMG3D4 software. It remesh both the volume and surface mesh of a tetrahedral mesh. It performs isotropic and anisotropic mesh adaptation and isovalue discretization of a level-set function.

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

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

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

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

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

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

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

## 6.6. MMG3D

### *Mmg3d*

KEYWORDS: Mesh - Anisotropic - Mesh adaptation

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

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

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

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

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

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

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

## 6.7. NOMESH

KEYWORDS: Mesh - Curved mesh - Tetrahedral mesh

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

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

## 6.8. ORComp

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

- Participants: Maria-Giovanna Rodio and Pietro-Marco Congedo
- Contact: Maria-Giovanna Rodio
- URL: <https://github.com/Orcomp/Orcomp>

## 6.9. RealfluidS

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

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

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

## 6.10. SH-COMP

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

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

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

## 6.11. SLOWS

*Shallow-water fLOWS*

KEYWORDS: Simulation - Free surface flows - Unstructured meshes

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

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

- Participants: Andrea Filippini, Luca Arpaia, Maria Kazolea, Mario Ricchiuto and Nikolaos Pattakos
- Contact: Mario Ricchiuto

## 6.12. Sparse-PDD

*Adaptive sparse polynomial dimensional decomposition for global sensitivity analysis*

KEYWORDS: Stochastic models - Uncertainty quantification

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

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

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

### 6.13. TUCWave

KEYWORD: Physical simulation

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

FUNCTIONAL DESCRIPTION: Fortran Planform which accounts for the study of near shore processes

- Participants: Argiris Delis, Ioannis Nikolos and Maria Kazolea
- Partner: CNRS
- Contact: Maria Kazolea

## DEFI Project-Team

# 5. New Software and Platforms

## 5.1. FVforBlochTorrey

- Participant: Jing Rebecca Li
- Contact: Jing Rebecca Li

## 5.2. InvGIBC

- Participant: Nicolas Chaulet
- Contact: Housseem Haddar

## 5.3. RODIN

FUNCTIONAL DESCRIPTION: In the framework of the RODIN project we continue to develop with our software partner ESI the codes Topolev and Geolev for topology and geometry shape optimization of mechanical structures using the level set method.

- Contact: Grégoire Allaire

## 5.4. samplings-2d

*This software solves forward and inverse problems for the Helmholtz equation in 2-D.*

FUNCTIONAL DESCRIPTION: 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

- Participant: Housseem Haddar
- Contact: Housseem Haddar
- URL: <http://sourceforge.net/projects/samplings-2d/>

## 5.5. Samplings-3d

FUNCTIONAL DESCRIPTION: 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.

- Contact: Housseem Haddar

## 5.6. SCILAB

SCIENTIFIC DESCRIPTION: Scilab includes hundreds of mathematical functions. It has a high level programming language allowing access to advanced data structures, 2-D and 3-D graphical functions.

A large number of functionalities is included in Scilab:

Maths & Simulation For usual engineering and science applications including mathematical operations and data analysis. 2-D & 3-D Visualization Graphics functions to visualize, annotate and export data and many ways to create and customize various types of plots and charts. Optimization Algorithms to solve constrained and unconstrained continuous and discrete optimization problems. Statistics Tools to perform data analysis and modeling Control System Design & Analysis Standard algorithms and tools for control system study Signal Processing Visualize, analyze and filter signals in time and frequency domains. Application Development Increase Scilab native functionalities and manage data exchanges with external tools. Xcos - Hybrid dynamic systems modeler and simulator Modeling mechanical systems, hydraulic circuits, control systems...

FUNCTIONAL DESCRIPTION: Scilab is free and open source software for numerical computation providing a powerful computing environment for engineering and scientific applications.

- Participant: Grégoire Allaire
- Contact: Grégoire Allaire
- URL: <http://www.scilab.org/>

## ECUADOR Project-Team

# 5. New Software and Platforms

## 5.1. AIRONUM

KEYWORDS: Computational Fluid Dynamics - Turbulence

FUNCTIONAL DESCRIPTION: Aironum is an experimental software that solves the unsteady compressible Navier-Stokes equations with k-epsilon, LES-VMS and hybrid turbulence modelling on parallel platforms, using MPI. The mesh model is unstructured tetrahedrization, with possible mesh motion.

- Participant: Alain Dervieux
- Contact: Alain Dervieux
- URL: <http://www-sop.inria.fr/tropics/aironum>

## 5.2. TAPENADE

KEYWORDS: Static analysis - Optimization - Compilation - Gradients

SCIENTIFIC DESCRIPTION: Tapenade implements the results of our research about models and static analyses for AD. Tapenade can be downloaded and installed on most architectures. Alternatively, it can be used as a web server. Higher-order derivatives can be obtained through repeated application.

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 analyses 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.

FUNCTIONAL DESCRIPTION: Tapenade is an Algorithmic Differentiation tool that transforms an original program into a new program that computes derivatives of the original program. Algorithmic 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, adjoint, and vector adjoint.

NEWS OF THE YEAR: - Continued development of multi-language capacity: AD of codes mixing Fortran and C - Creation of a front-end for C++ based on Clang - Improved support for the current frontiers of Source-Transformation AD: Dynamic Memory, and MPI

- Participants: Benoît Dufumier, Louis Becquey, Laurent Hascoët and Valérie Pascual
- Contact: Laurent Hascoët
- URL: <http://www-sop.inria.fr/tropics/tapenade.html>

## GAMMA3 Project-Team

### 3. New Software and Platforms

#### 3.1. ABL4FLO

KEYWORDS: Boundary layers - Hybrid meshes

FUNCTIONAL DESCRIPTION: ABL4FLO is designed to generate 3D adapted boundary layer meshes by using a cavity-based operator.

- Participant: Adrien Loseille
- Contact: Adrien Loseille

#### 3.2. AMA4FLO

*Anisotropic Mesh Adaptation 4 FLOW*

KEYWORDS: 3D - Mesh adaptation

FUNCTIONAL DESCRIPTION: 3D, surface, 2D anisotropic mesh generation

- Participant: Adrien Loseille
- Contact: Adrien Loseille
- URL: <http://pages.saclay.inria.fr/adrien.loseille/index.php?page=softwares>

#### 3.3. BL2D

KEYWORDS: Abstraction - Meshing - Isotropic - Anisotropic - Delaunay

FUNCTIONAL DESCRIPTION: This software package stems from a former one called BL2D-V1. The meshing method is of controlled Delaunay type, isotropic or anisotropic. The internal point generation follows a frontal logic, and their connection is realised as in a classical Delaunay approach. Quadrilaterals are obtained by a pairing process. The direct construction of degree 2 element has been made possible via the control of the domain boundary mesh, in order to ensure the desired compatibility. The boundary middle nodes are located according to the curvilinear abscissa. The internal middle nodes are, by default, at the middle of the corresponding edges.

RELEASE FUNCTIONAL DESCRIPTION: Par rapport à la version V1, il offre de nombreuses possibilités nouvelles : méthode frontale, triangles quadratiques courbes, quadrilatères de degré 1 ou 2, frontières déformables, allocation dynamique de mémoire, etc

- Participants: Houman Borouchaki and Patrick Laug
- Contact: Patrick Laug
- URL: <http://pages.saclay.inria.fr/patrick.laug/logiciels/bl2d-v2/INDEX.html>

#### 3.4. BL2D-ABAQ

KEYWORDS: Anisotropic - Delaunay - Automatic mesher

FUNCTIONAL DESCRIPTION: The meshing method is the same as BL2D in an adaptive process. An a posteriori error estimation of a solution at the nodes of the current mesh results in a size map. A new mesh satisfying these size specifications (made continuous) is built, and the solution is interpolated on the new mesh.

- Participants: Abel Cherouat, Houman Borouchaki and Patrick Laug
- Contact: Patrick Laug

### 3.5. BLGEOL

KEYWORDS: Automatic mesher - Geologic structure

FUNCTIONAL DESCRIPTION: BLGEOL-V1 software can generate hex-dominant meshes of geologic structures complying with different geometric constraints: surface topography (valleys, reliefs, rivers), geologic layers and underground workings. First, a reference 2D domain is obtained by projecting all the line constraints into a horizontal plane. Different size specifications are given for rivers, outcrop lines and workings. Using an adaptive methodology, the size variation is bounded by a specified threshold in order to obtain a high quality quad-dominant mesh. Secondly, a hex-dominant mesh of the geological medium is generated by a vertical extrusion, taking into account the surfaces found (interfaces between two layers, top or bottom faces of underground workings). The generation of volume elements follows a global order established on the whole set of surfaces to ensure the conformity of the resulting mesh.

- Participants: Houman Borouchaki and Patrick Laug
- Contact: Patrick Laug
- URL: <https://team.inria.fr/gamma3/project-presentation/gamma-software/>

### 3.6. BLMOL

KEYWORDS: Mesher - Molecular surface

SCIENTIFIC DESCRIPTION: An increasingly important part of quantum chemistry is devoted to molecular surfaces. To model such a surface, each constituting atom is idealized by a simple sphere. Surface mesh generation techniques are then used either for visualization or for simulation, where mesh quality has a strong influence on solution accuracy. First, a boundary representation (B-rep) of the surface is obtained, i.e. a set of patches and the topological relations between them. Second, an appropriate parameterization and a metric map are computed for each patch. Third, meshes of the parametric domains are generated with respect to an induced metric map, using a combined advancing-front generalized-Delaunay approach. Finally these meshes are mapped onto the entire surface. Several application examples illustrate various capabilities of our method.

FUNCTIONAL DESCRIPTION: BLMOL is a molecular surface mesher.

- Participants: Houman Borouchaki and Patrick Laug
- Contact: Patrick Laug
- URL: <http://pages.saclay.inria.fr/patrick.laug/logiciels/blmol/INDEX.html>

### 3.7. BLSURF

KEYWORDS: Automatic mesher - Molecular surface

FUNCTIONAL DESCRIPTION: An indirect method for meshing parametric surfaces conforming to a user-specifiable size map is used. First, from this size specification, a Riemannian metric is defined so that the desired mesh is one with unit length edges with respect to the related Riemannian space (the so-called

- Participants: Houman Borouchaki and Patrick Laug
- Partner: Université de Technologie de Troyes
- Contact: Patrick Laug
- URL: <https://team.inria.fr/gamma3/project-presentation/gamma-software/>

### 3.8. FEFLOA-REMESH

KEYWORDS: Scientific calculation - Anisotropic - Mesh adaptation

FUNCTIONAL DESCRIPTION: FEFLOA-REMESH is intended to generate adapted 2D, surface and volume meshes by using a unique cavity-based operator. The metric-aligned or metric-orthogonal approach is used to generate high quality surface and volume meshes independently of the anisotropy involved.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Adrien Loseille
- URL: <http://pages.saclay.inria.fr/adrien.loseille/index.php?page=softwares>

### 3.9. GAMANIC 3D

KEYWORDS: Tetrahedral mesh - Delaunay - Anisotropic size and direction control - Automatic mesher

FUNCTIONAL DESCRIPTION: GAMANIC3D is a volume mesher governed by a (anisotropic) size and directional specification metric field.

- Participants: Adrien Loseille, Éric Saltel, Frédéric Alauzet, Frederic Hecht, Houman Borouchaki and Paul Louis George
- Contact: Paul Louis Georges
- URL: <http://www.meshgems.com/volume-meshing.html>

### 3.10. GAMHIC 3D

KEYWORDS: Tetrahedral mesh - Delaunay - Isotropic - Automatic mesher

FUNCTIONAL DESCRIPTION: GAMHIC3D is a volume mesher governed by a (isotropic) size specification metric field.

- Participants: Adrien Loseille, Éric Saltel, Frédéric Alauzet, Frederic Hecht, Houman Borouchaki and Paul Louis George
- Contact: Paul Louis George
- URL: <http://www.meshgems.com/volume-meshing.html>

### 3.11. GHS3D

KEYWORDS: Tetrahedral mesh - Delaunay - Automatic mesher

FUNCTIONAL DESCRIPTION: GHS3D is an automatic volume mesher

- Participants: Adrien Loseille, Éric Saltel, Frédéric Alauzet, Frederic Hecht, Houman Borouchaki and Paul Louis George
- Contact: Paul Louis George
- URL: <http://www.meshgems.com/volume-meshing.html>

### 3.12. HEXOTIC

KEYWORDS: 3D - Mesh generation - Meshing - Unstructured meshes - Octree/Quadtree - Multi-threading - GPGPU - GPU

FUNCTIONAL DESCRIPTION: Input: a triangulated surface mesh and an optional size map to control the size of inner elements.

Output: a fully hexahedral mesh (no hybrid elements), valid (no negative jacobian) and conformal (no dangling nodes) whose surface matches the input geometry.

The software is a simple command line that requires no knowledge on meshing. Its arguments are an input mesh and some optional parameters to control elements sizing, curvature and subdomains as well as some features like boundary layers generation.

- Participant: Loïc Maréchal
- Partner: Distene
- Contact: Loïc Maréchal
- URL: <https://team.inria.fr/gamma3/project-presentation/gamma-software/hexotic/>

### 3.13. Nimbus 3D

KEYWORDS: Surface reconstruction - Point cloud

FUNCTIONAL DESCRIPTION: Nimbus3D is a surface reconstruction method piece of software

- Participants: Houman Borouchaki and Paul Louis George
- Contact: Paul Louis George
- URL: <http://www.meshgems.com/volume-meshing.html>

### 3.14. VIZIR

*Maillages Clés en Main pour la Simulation Numérique*

KEYWORD: Mesh

FUNCTIONAL DESCRIPTION: VIZIR is intended to visualize and modify interactively simplicial, hybrid and high order curved meshes.

- Participants: Adrien Loseille, Alexis Loyer and Julien Castelneau
- Contact: Adrien Loseille
- URL: <http://pages.saclay.inria.fr/adrien.loseille/index.php?page=softwares>

### 3.15. Wolf

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Numerical solver for the Euler and compressible Navier-Stokes equations with turbulence modelling. ALE formulation for moving domains. Modules of interpolation, mesh optimisation and moving meshes. Wolf is written in C++, and may be later released as an opensource library. FELiScE was registered in July 2014 at the Agence pour la Protection des Programmes under the Inter Deposit Digital Number IDDN.FR.001.340034.000.S.P.2014.000.10000.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.16. Wolf-Bloom

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-Bloom is a structured boundary layer mesh generator using a pushing approach. It start from an existing volume mesh and insert a structured boundary layer by pushing the volume mesh. The volume mesh deformation is solved with an elasticity analogy. Mesh-connectivity optimizations are performed to control volume mesh element quality.

- Participants: Adrien Loseille, David Marcum and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.17. Wolf-Elast

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-Elast is a linear elasticity solver using the P1 Finite-Element method. The Young and Poisson coefficient can be parametrized. The linear system is solved using the Conjugate Gradient method with the LUSGS preconditioner.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.18. Wolf-Interpol

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-Interpol is a tool to transfer scalar, vector and tensor fields from one mesh to another one. Polynomial interpolation (from order 2 to 4) or conservative interpolation operators can be used. Wolf-Interpol also extract solutions along lines or surfaces.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.19. Wolf-MovMsh

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-MovMsh is a moving mesh algorithm coupled with mesh-connectivity optimization. Mesh deformation is computed by means of a linear elasticity solver or a RBF interpolation. Smoothing and swapping mesh optimization are performed to maintain good mesh quality. It handles rigid bodies or deformable bodies, and also rigid or deformable regions of the domain.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Paul Louis George
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.20. Wolf-Nsc

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-Nsc is numerical flow solver solving steady or unsteady turbulent compressible Euler and Navier-Stokes equations. The available turbulent models are the Spalart-Almaras and the Menter SST k-omega. A mixed finite volume - finite element numerical method is used for the discretization. Second order spatial accuracy is reached thanks to MUSCL type methods. Explicit or implicit time integration are available. It also resolved dual (adjoint) problem and compute error estimate for mesh adaptation.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

### 3.21. Wolf-Spyder

KEYWORD: Scientific calculation

FUNCTIONAL DESCRIPTION: Wolf-Spyder is a metric-based mesh quality optimizer using vertex smoothing and edge/face swapping.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: [https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code\\_eng.html](https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html)

**IPSO Project-Team (section vide)**

## **MATHERIALS Project-Team**

# **6. New Software and Platforms**

## **6.1. simol**

KEYWORDS: Molecular simulation - Quantum chemistry - Statistical physics - C++ - OpenMP

FUNCTIONAL DESCRIPTION: Molecular simulation software written in C++

- Contact: Gabriel Stoltz

## MEMPHIS Project-Team

## 6. New Software and Platforms

### 6.1. COCOFLOW

KEYWORDS: 3D - Elasticity - MPI - Compressible multimaterial flows

FUNCTIONAL DESCRIPTION: The code is written in fortran 95 with a MPI parallelization. It solves equations of conservation modeling 3D compressible flows with elastic models as equation of state.

- Contact: Florian Bernard
- URL: <https://gforge.inria.fr/projects/cocoflow>

### 6.2. KOPPA

*Kinetic Octree Parallel PolyAtomic*

FUNCTIONAL DESCRIPTION: KOPPA is a C++/MPI numerical code solving a large range of rarefied flows from external to internal flows in 1D, 2D or 3D. Different kind of geometries can be treated such as moving geometries coming from CAO files or analytical geometries. The models can be solved on Octree grids with dynamic refinement.

- Participant: Florian Bernard
- Contact: Florian Bernard
- URL: <https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary>

### 6.3. NaSCar

*Navier-Stokes Cartesian*

KEYWORDS: HPC - Numerical analyse - Fluid mechanics - Langage C - PETSc

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

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

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

- Participant: Michel Bergmann
- Contact: Michel Bergmann
- URL: <https://gforge.inria.fr/projects/nascar/>

### 6.4. NS-penal

*Navier-Stokes-penalization*

KEYWORDS: 3D - Incompressible flows - 2D

FUNCTIONAL DESCRIPTION: The software can be used as a black box with the help of a data file if the obstacle is already proposed. For new geometries the user has to define them. It can be used with several boundary conditions (Dirichlet, Neumann, periodic) and for a wide range of Reynolds numbers.

- Partner: Université de Bordeaux
- Contact: Charles-Henri Bruneau

**MEPHYSTO Project-Team (section vide)**

## **MOKAPLAN Project-Team**

## **5. New Software and Platforms**

### **5.1. ALG2**

FUNCTIONAL DESCRIPTION: ALG2 for Monge Mean-Field Games, Monge problem and Variational problems under divergence constraint. A generalisation of the ALG2 algorithm has been implemented in FreeFem++.

- Contact: Jean-David Benamou
- URL: <https://team.inria.fr/mokaplan/augmented-lagrangian-simulations/>

### **5.2. Mokabajour**

FUNCTIONAL DESCRIPTION: We design a software resolving the following inverse problem: define the shape of a mirror which reflects the light from a source to a defined target, distribution and support of densities being prescribed. Classical applications include the conception of solar oven, public lightning, car headlights. . . Mathematical modeling of this problem, related to the optimal transport theory, takes the form of a nonlinear Monge-Ampere type PDE. The numerical resolution of these models remained until recently a largely open problem. MOKABAJOUR project aims to develop, using algorithms invented especially at Inria and LJK, a reflector design software more efficient than geometrical methods used so far. The final step is to realize and physically test prototype reflectors.

- Participants: Boris Thibert, Jean-David Benamou and Quentin Mérigot
- Contact: Jean-David Benamou
- URL: <https://project.inria.fr/mokabajour/>

### **5.3. Platforms**

#### **5.3.1. MABV2**

A 2D Julia implementation of the algorithm described in [25]. [https://gforge.inria.fr/scm/browser.php?group\\_id=9995](https://gforge.inria.fr/scm/browser.php?group_id=9995)

## NACHOS Project-Team

# 5. New Software and Platforms

## 5.1. DIOGENeS

*Discontinuous Galerkin Nanoscale Solvers*

KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin - Computational nanophotonics

FUNCTIONAL DESCRIPTION: DIOGENeS relies on a two layer architecture. The core of the suite is a library of generic software components (data structures and algorithms) for the implementation of high order DG (Discontinuous Galerkin) and HDG (Hybridizable Discontinuous Galerkin) schemes formulated on unstructured tetrahedral and hybrid structured/unstructured (cubic/tetrahedral) meshes. This library is used to develop dedicated simulation software for time-domain and frequency-domain problems relevant to nanophotonics and nanoplasmonics, considering various material models.

- Contact: Stéphane Lanteri
- URL: <http://www-sop.inria.fr/nachos/index.php/Software/DIOGENeS>

## 5.2. GERShWIN

*discontinuous Galerkin Solver for microWave Interaction with biological tissues*

KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin - Computational bioelectromagnetics

FUNCTIONAL DESCRIPTION: GERShWIN is based on a high order DG method formulated on unstructured tetrahedral meshes for solving the 3D system of time-domain Maxwell equations coupled to a Debye dispersion model.

- Contact: Stéphane Lanteri
- URL: <http://www-sop.inria.fr/nachos/index.php/Software/GERShWIN>

## 5.3. HORSE

*High Order solver for Radar cross Section Evaluation*

KEYWORDS: High-Performance Computing - Computational electromagnetics - Discontinuous Galerkin

FUNCTIONAL DESCRIPTION: HORSE is based on a high order HDG (Hybridizable Discontinuous Galerkin) method formulated on unstructured tetrahedral and hybrid structured/unstructured (cubic/tetrahedral) meshes for the discretization of the 3D system of frequency-domain Maxwell equations, coupled to domain decomposition solvers.

- Contact: Stéphane Lanteri
- URL: <http://www-sop.inria.fr/nachos/index.php/Software/HORSE>

## NANO-D Project-Team

### 4. New Software and Platforms

#### 4.1. SAMSON

*Software for Adaptive Modeling and Simulation Of Nanosystems*

KEYWORDS: Structural Biology - Nanosystems - Simulation - Bioinformatics - Chemistry

SCIENTIFIC DESCRIPTION: Please refer to <https://www.samson-connect.net>

FUNCTIONAL DESCRIPTION: SAMSON is a software platform for real-time modelling and simulation of natural or artificial nanosystems. 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.).

- Contact: Stéphane Redon
- URL: <http://nano-d.inrialpes.fr/software/>

#### 4.2. HermiteFit

*A new docking algorithm for rapid fitting atomic structures into cryo-EM density maps*

FUNCTIONAL DESCRIPTION: HermiteFit is a new docking algorithm for rapid fitting atomic structures into cryo-EM density maps using 3D orthogonal Hermite functions. HermiteFit uses the cross-correlation or the Laplacian-filtered cross-correlation as the fitting criterion. HermiteFit exhaustively rotates the protein density in the Hermite space and then converts the expansion coefficients into the Fourier space for the subsequent fast FFT-based correlation computations.

- Partners: IBS - FZJ Juelich
- Contact: Sergey Grudinin
- URL: <https://team.inria.fr/nano-d/software/hermitefit/>

#### 4.3. Knodle

*KNOWledge-Driven Ligand Extractor*

FUNCTIONAL DESCRIPTION: KNOWledge-Driven Ligand Extractor is a software library for the recognition of atomic types, their hybridization states and bond orders in the structures of small molecules. Its prediction model is based on nonlinear Support Vector Machines. The process of bond and atom properties perception is divided into several steps. At the beginning, only information about the coordinates and elements for each atom is available :

Connectivity is recognized. A search of rings is performed to find the Smallest Set of Smallest Rings (SSSR). Atomic hybridizations are predicted by the corresponding SVM model. Bond orders are predicted by the corresponding SVM model. Aromatic cycles are found. Atomic types are set in obedience to the functional groups. Some bonds are reassigned during this stage.

- Partner: MIPT Moscow
- Contact: Sergey Grudinin
- URL: <https://team.inria.fr/nano-d/software/Knodle/>

#### 4.4. RigidRMSD

*A library for rapid computations of the root mean square deviations (RMSDs) corresponding to a set of rigid body transformations of a coordinate vector*

FUNCTIONAL DESCRIPTION: RigidRMSD is a library for rapid computations of the root mean square deviations (RMSDs) corresponding to a set of rigid body transformations of a coordinate vector (which can be a molecule in PDB format, for example). Calculation of the RMSD splits into two steps:

Initialization, which is linear in the number of vector entities (or particles in a rigid body). RMSD computation, which is computed in constant time for a single rigid-body spatial transformation (rotation + translation). This step uses the inertia tensor and the the center of mass computed on the first step. Initialization step is performed only once. It makes RigidRMSD particularly useful when computing multiple RMSDs, since each new RMSD calculation takes only constant time.

- Contact: Sergey Grudinin
- URL: <https://team.inria.fr/nano-d/software/rigidrmsd/>

## 4.5. DockTrina

*A novel protein docking method for modeling the 3D structures of nonsymmetrical triangular trimers*

FUNCTIONAL DESCRIPTION: DockTrina is a novel protein docking method for modeling the 3D structures of nonsymmetrical triangular trimers. The method takes as input pair-wise contact predictions from a rigid body docking program. It then scans and scores all possible combinations of pairs of monomers using a very fast root mean square deviation (RMSD) test (see below). Finally, it ranks the predictions using a scoring function which combines triples of pair-wise contact terms and a geometric clash penalty term. The overall approach takes less than 2 min per complex on a modern desktop computer.

- Contact: Sergey Grudinin
- URL: <https://team.inria.fr/nano-d/software/docktrina/>

## POEMS Project-Team

# 6. New Software and Platforms

## 6.1. COFFEE

FUNCTIONAL DESCRIPTION: COFFEE is a 3D BEM-accelerated FMM solver for linear elastodynamics (full implementation, 30 000 lines of Fortran 90). The 3-D elastodynamic equations are solved with the boundary element method accelerated by the multi-level fast multipole method. The fundamental solutions for the infinite space are used in this implementation. A boundary element-boundary element coupling strategy is also implemented so multi-region problems (strata inside a valley for example) can be solved.

- Contact: Stéphanie Chaillat

## 6.2. XLiFE++

FUNCTIONAL DESCRIPTION: XLiFE++ is a Finite Element library in C++ based on philosophy of the previous library Melina in Fortran but with new capabilities (boundary elements, discontinuous Galerkin methods, more integrated tools -in particular mesh tools - and high performance computing skills, multithread and GPU computation).

- Contact: Eric Lunéville

**RAPSODI Project-Team (section vide)**

**APICS Project-Team (section vide)**

## BIPOP Project-Team

## 6. New Software and Platforms

### 6.1. ACEF

*Automatic switched Circuits Equation Formualtion*

KEYWORDS: Simulation - Electrical circuit - Switched systems

SCIENTIFIC DESCRIPTION: Nonsmooth Modeling and Simulation for Switched Circuits concerns the modeling and the numerical simulation of switched circuits with the nonsmooth dynamical systems (NSDS) approach, using piecewise-linear and multivalued models of electronic devices like diodes, transistors, switches. Numerous examples (ranging from introductory academic circuits to various types of power converters) are analyzed and many simulation results obtained with the Inria open-source SICONOS software package are presented. Comparisons with SPICE and hybrid methods demonstrate the power of the NSDS approach. Nonsmooth Modeling and Simulation for Switched Circuits is intended to researchers and engineers in the field of circuits simulation and design, but may also attract applied mathematicians interested by the numerical analysis for nonsmooth dynamical systems, as well as researchers from Systems and Control.

References: Nonsmooth Modeling and Simulation for Switched Circuits Authors: Acary, Vincent, Bonnefon, Olivier, Brogliato, Bernard (<http://www.springer.com/fr/book/9789048196807>)

FUNCTIONAL DESCRIPTION: The Automatic Circuit Equations Formulation (ACEF) module is the implementation of the automatic circuit equation extended to general nonsmooth components. From a SPICE netlist, possibly augmented by some nonsmooth components, the ACEF builds a dynamical formulation that can be simulated by SICONOS.

- Participants: Olivier Bonnefon and Vincent Acary
- Contact: Vincent Acary
- URL: <http://bipop.inrialpes.fr/people/acary/>

### 6.2. Approche

KEYWORD: Geometric computing

- Participants: Alexandre Derouet-Jourdan, Florence Descoubes and Joëlle Thollot
- Contact: Florence Descoubes
- URL: <http://bipop.inrialpes.fr/~bertails/Papiers/floatingTangents3d.html>

### 6.3. CloC

*Super Space Clothoids in C*

KEYWORD: Physical simulation

FUNCTIONAL DESCRIPTION: Reference software implementing the paper "Super Space Clothoids", R. Casati and F. Bertails-Descoubes, ACM Transactions on Graphics, 2013

- Participants: Florence Descoubes and Romain Casati
- Partner: UJF
- Contact: Florence Descoubes
- URL: <http://bipop.inrialpes.fr/people/casati/publications/codes/ssc.html>

### 6.4. MECHE-COSM

*Modeling Entangled fiber with frictional Contact in Hair*

KEYWORDS: Physical simulation - Frictional contact - Thin elastic rod

FUNCTIONAL DESCRIPTION: Implements super-helices [Bertails et al. 2006] coupled together by a hybrid algorithm for frictional contact [Daviet et al. 2011].

- Participants: Florence Bertails Descoubes, Florent Cadoux and Gilles Daviet
- Contact: Florence Descoubes

## 6.5. N1cv2

KEYWORDS: Optimization - Decomposition

- Participants: Claude Lemaréchal and Claudia Sagastizabal
- Partners: Université fédérale de Rio de Janeiro - Université de Varsovie - Université de Washington - Université de Pise
- Contact: Jérôme Malick
- URL: <http://www.inrialpes.fr/bipop/>

## 6.6. SALADYN MULTIBODY

KEYWORDS: Physical simulation - Co-simulation

FUNCTIONAL DESCRIPTION: The project SALADYN aims at designing and implementing a new software platform into Salomé-Méca by coupling three kinds of mechanical models: a) Deformable bodies, mainly through their finite element representation, b) rigid multi-body systems and c) multi-contact systems. The goal is to obtain a close coupling of these models for the modeling and the simulation in a nonsmooth dynamical framework, able to deal rigorously with the unilateral contact and Coulomb's friction. This platform will be composed by the integration of the following components:

Salomé. An OpenSource platform for the pre and post-processing and the coupling of numerical software codes. Code\_Aster. An OpenSource Finite Element Application, which has already been integrated in Salomé, under the name of Salomé-méca. LMGC90. An OpenSource software for the modeling and the simulation of multicontact systems. Siconos. An OpenSource software for the modeling, the simulation and the control of nonsmooth Dynamical systems Besides this integration, the main deliverable of this project is a common numerical software which allows the interoperability of the models through a multiple representation of an unique physical object, and a dynamic adaptability in time based on the user needs and the simulation requirements (accuracy, efficiency, abstraction, etc.). The consortium (Schneider Electric, EDF, Inria, LMGC, LAMSID) brings together well-recognized skills of academic laboratories and companies, which possess a strong experience in structural analysis and dynamical analysis in the field of nonsmooth dynamics. The industrial partners will provide the project with effective test-beds and experiments, which will be very reliable element for validation and performance analysis. The expected result of this project should concern a large field of application ranging from transport, energy, micro-mechanical systems to divided materials such as Masonry or granular matter.

More generally, one aim of this project is to federate the national academic and industrial community for the design and the simulation of complex mechanical in non smooth interactions into a common OpenSource software platform.

- Participants: Olivier Bonnefon and Vincent Acary
- Contact: Vincent Acary
- URL: <http://saladyn.gforge.inria.fr>

## 6.7. SICONOS

*Modeling, simulation and control of nonsmooth dynamical systems*

KEYWORDS: Friction - Collision - SD - DCDC - MEMS - NSDS - Mechanical multi-body systems

FUNCTIONAL DESCRIPTION: Siconos is an open-source scientific software primarily targeted at modeling and simulating nonsmooth dynamical systems in C++ and in Python: - Mechanical systems (rigid or solid) with unilateral contact and Coulomb friction and impact (nonsmooth mechanics, contact dynamics, multibody systems dynamics or granular materials). - Switched Electrical Circuit such as electrical circuits with ideal and piecewise linear components: power converter, rectifier, Phase-Locked Loop (PLL) or Analog-to-Digital converter. - Sliding mode control systems. - Biology (Gene regulatory network). Other applications are found in Systems and Control (hybrid systems, differential inclusions, optimal control with state constraints), Optimization (Complementarity systems and Variational inequalities), Fluid Mechanics, and Computer Graphics.

- Participants: Franck P rignon, Maurice Br mond, Olivier Bonnefon and Vincent Acary
- Contact: Vincent Acary
- URL: <http://siconos.gforge.inria.fr>

## 6.8. Platforms: SICONOS

### 6.8.1. Platform A : SICONOS

**Participants:** Vincent Acary, Maurice Br mond, Olivier Huber, Franck P rignon.

In the framework of the FP5 European project Siconos (2002-2006), Bipop was the leader of the Work Package 2 (WP2), dedicated to the numerical methods and the software design for nonsmooth dynamical systems. This has given rise to the platform SICONOS which is the main software development task in the team. 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, interconnections, 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/MECHANICS. 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 between B-Rep description and on Bullet for contact detection between meshes.

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

## COMMANDS Project-Team

# 6. New Software and Platforms

## 6.1. BOCOP

*Boîte à Outils pour le Contrôle Optimal*

KEYWORDS: Dynamic Optimization - Identification - Biology - Numerical optimization - Energy management - Transportation

FUNCTIONAL DESCRIPTION: Bocop is 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, energy and biology. Bocop includes a module for parameter identification and a graphical interface, and runs under Linux / Windows / Mac.

RELEASE FUNCTIONAL DESCRIPTION: Handling of delay systems Alternate automatic differentiation tool: CppAD Update for CMake and MinGW (windows version)

- Participants: Benjamin Heymann, Virgile Andreani, Jinyan Liu, Joseph Frédéric Bonnans and Pierre Martinon
- Contact: Pierre Martinon
- URL: <http://bocop.org>

## 6.2. Bocop HJB

KEYWORDS: Optimal control - Stochastic optimization - Global optimization

FUNCTIONAL DESCRIPTION: Toolbox for stochastic or deterministic optimal control, dynamic programming / HJB approach.

RELEASE FUNCTIONAL DESCRIPTION: User interface State jumps for switched systems Explicit handling of final conditions Computation of state probability density (fiste step to mean field games)

- Participants: Benjamin Heymann, Jinyan Liu, Joseph Frédéric Bonnans and Pierre Martinon
- Contact: Joseph Frédéric Bonnans
- URL: <http://bocop.org>

## 6.3. Bocop Avion

KEYWORDS: Optimization - Aeronautics

FUNCTIONAL DESCRIPTION: Optimize the climb speeds and associated fuel consumption for the flight planning of civil airplanes.

NEWS OF THE YEAR: Improved atmosphere model 2D interpolations for temperature and wind data

- Participants: Gregorutti Baptiste, Cindie Andrieu, Anamaria Lupu, Joseph Frédéric Bonnans, Karim Tekkal, Pierre Jouniaux and Pierre Martinon
- Partner: Safety Line
- Contact: Pierre Martinon
- URL: <http://www.safety-line.fr>

## 6.4. Bocop HJB Avion

KEYWORDS: Optimization - Aeronautics

FUNCTIONAL DESCRIPTION: Optimize the climb and cruising trajectory of flight by a HJB approach.

NEWS OF THE YEAR: First demonstrator for cruise flight deployed at Safety Line

- Participants: Pierre Martinon, Joseph Frédéric Bonnans, Jinyan Liu, Gregorutti Baptiste and Anamaria Lupu
- Partner: Safety Line
- Contact: Pierre Martinon
- URL: <http://www.safety-line.fr>

## DISCO Project-Team

# 6. New Software and Platforms

## 6.1. YALTA

### *Yet Another LTI TDS Algorithm*

FUNCTIONAL DESCRIPTION: The YALTA toolbox is a Matlab toolbox 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 and on classical continuation methods exploiting the particularities of the problem.

- Participants: André Fioravanti, Catherine Bonnet, David Avanesoff, Hugo Cavallera, Jim Pioche and Le Ha Vy Nguyen
- Contact: Catherine Bonnet
- URL: <http://yalta-toolbox.gforge.inria.fr/>

## **GECO Project-Team**

# **6. New Software and Platforms**

## **6.1. IRHD**

### *Image Reconstruction via Hypoelliptic Diffusion*

FUNCTIONAL DESCRIPTION: IRHD is a software for reconstruction of corrupted and damaged images. One of the main features of the algorithm on which the software is based is that it does not require any information about the location and character of the corrupted places. 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.

- Contact: Mario Sigalotti

## I4S Project-Team

## 6. New Software and Platforms

### 6.1. PEGASE

*Plate-forme Experte Générique pour Applications Sans-fil Embarquées*

KEYWORD: SHM (Structural Health Monitoring)

FUNCTIONAL DESCRIPTION: PEGASE is a generic high level wireless sensor platform. The main characteristics of PEGASE to reach this genericity are obtained by :

- Software genericity: use of a Linux embedded OS to make any developed application independent from the hardware, and to enable the user to manage the system without any physical operations.
- Hardware genericity: with a principle of daughter and mother boards, each redundant need is embedded (processing, memory, timing, GPS, energy, etc) where each pluggable daughter board implements a specific function (e.g., sensing, 3G, Lora/Sigfox and Ethernet wireless communications, signal processing and relay control).
- Accurate time synchronization: based on an original GPS and PPS algorithm, PEGASE platform is one of few boards able to time-stamp data from sensors or any event with an accuracy of some micro-seconds Universal Time.

After the industrial exploitation of PEGASE 1 (hundreds are sold), PEGASE 2 and the future PEGASE 3 version maintain and extend the previous platform. Focus on main characteristics is subject of electronic research and development:

- embed a "Debian" Linux operating system able to be validated for critical applications (such as SHM applications)
- embed a module dedicated to energy autonomy, to harvest energy from solar cells while considering the dis/charge of Lithium battery
- integrate a 3D accelerometer based on a MEMs to propose motion applications (train detection by vibration for example)
- new original daughter boards for new wireless IOT industrial protocols: LorA and Sigfox
- convert the proposed SDK (Single Development Kit) fully from C to C++ language
- a generic embedded front-end development called Zeus able to manage time control of Linux enslaved to the UTC synchronization, applications manager, network manager (from WiFi, Lora to 3G...), ...

Since 2017, PEGASE 2 platform is also used as the support for some lectures given at University of Nantes.

Associated to PEGASE hardware platform, I4S has also designed and programmed a generic Cloud Supervisor that allows to manage wireless sensors. In 2017 this application has matured, and has been licensed to two companies for industrial exploitation and distribution (Stimio and Power-Lan).

- Participants: Laurent Mevel, Mathieu Le Pen, Michael Doehler and Vincent Le Cam
- Contact: Michael Doehler
- URL: [http://www.a3ip.com/joomla/index.php?option=com\\_content&view=article&id=12&Itemid=8](http://www.a3ip.com/joomla/index.php?option=com_content&view=article&id=12&Itemid=8)

### 6.2. TrackingMecaSysEvo

KEYWORDS: Particular filter - Kalman filter - Monte-Carlo - Bayesian estimation - Vibrating system

FUNCTIONAL DESCRIPTION: Based on a IPKF (Interacting Particles and Kalman Filter) implementation, TrackingMecaSysEvo allow mechanical parameters tracking over the time for a 1-2-3D vibrating model. The algorithm insure also, input force and ambient noise estimation

- Participants: Antoine Crinière, Laurent Mevel and Subhamoy Sen
- Partner: IFSTTAR
- Contact: Laurent Mevel

## MCTAO Project-Team

# 5. New Software and Platforms

## 5.1. Hampath

KEYWORDS: Optimal control - Second order conditions - Differential homotopy - Ordinary differential equations

FUNCTIONAL DESCRIPTION: Hampath is a software developed to solve optimal control problems by a combination of Hamiltonian et path following methods. Hampath includes shooting and computation of conjugate points. It is an evolution of the software cotcot ([apo.enseeiht.fr/cotcot](http://apo.enseeiht.fr/cotcot)). It has a Fortran kernel, uses Tapenade ([www-sop.inria.fr/tropics/tapenade.html](http://www-sop.inria.fr/tropics/tapenade.html)) for automatic differentiation and has a Matlab interface.

- Participants: Jean-Baptiste Caillau, Joseph Gergaud and Olivier Cots
- Contact: Jean-Baptiste Caillau
- URL: <http://www.hampath.org>

## NECS Project-Team

## 6. New Software and Platforms

### 6.1. GTL

#### *Grenoble Traffic Lab*

**FUNCTIONAL DESCRIPTION:** The Grenoble Traffic Lab (GTL) initiative, led by the NeCS team, is a real-time traffic data Center (platform) that collects traffic road infrastructure information in real-time with minimum latency and fast sampling periods. The main elements of the GTL are: a real-time data-base, a show room, and a calibrated micro-simulator of the Grenoble South Ring. Sensed information comes from a dense wireless sensor network deployed on Grenoble South Ring, 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. In addition to real data, the project also uses simulated data, in order to validate models and to test the ramp-metering, the micro-simulator is a commercial software (developed by TSS AIMSUN ©). More details at <http://necs.inrialpes.fr/pages/grenoble-traffic-lab.php>

- Participants: Alain Kibangou, Andres Alberto Ladino Lopez, Anton Andreev, Carlos Canudas-De-Wit, Dominik Pisarski, Enrico Lovisari, Fabio Morbidi, Federica Garin, Hassen Fourati, Iker Bellicot, Maria Laura Delle Monache, Paolo Frasca, Pascal Bellemain, Pietro Grandinetti, Rémi Piotaix, Rohit Singhal and Vadim Bertrand
- Contact: Carlos Canudas-De-Wit
- URL: <http://necs.inrialpes.fr/pages/grenoble-traffic-lab.php>

### 6.2. Benchmarks Attitude Smartphones

**KEYWORDS:** Performance analysis - Sensors - Motion analysis - Experimentation - Smartphone

**SCIENTIFIC DESCRIPTION:** We investigate the precision of attitude estimation algorithms in the particular context of pedestrian navigation with commodity smartphones and their inertial/magnetic sensors. We report on an extensive comparison and experimental analysis of existing algorithms. We focus on typical motions of smartphones when carried by pedestrians. We use a precise ground truth obtained from a motion capture system. We test state-of-the-art attitude estimation techniques with several smartphones, in the presence of magnetic perturbations typically found in buildings. We discuss the obtained results, analyze advantages and limits of current technologies for attitude estimation in this context. Furthermore, we propose a new technique for limiting the impact of magnetic perturbations with any attitude estimation algorithm used in this context. We show how our technique compares and improves over previous works.

- Participants: Hassen Fourati, Nabil Layaïda, Pierre Genevès and Thibaud Michel
- Partner: GIPSA-Lab
- Contact: Pierre Genevès
- URL: <http://tyrex.inria.fr/mobile/benchmarks-attitude/>

### 6.3. GreAR

#### *Grenoble AR-Tour based on geolocation.*

**KEYWORDS:** Augmented reality - Geolocation - Smartphone

**FUNCTIONAL DESCRIPTION:** This application is an AR navigator specifically designed for pedestrians. This application was initially developed during the Venturi FP7 (2011-2015) project and has been updated with our AR framework since then. Between two visually driven AR experiences (at the time, developed by partners), the navigator provides the user with an audio and visual guidance through a pre-defined touristic path in Grenoble. The position of the user is obtained through a fusion of GPS signal (when available), pedometer estimates and a map-matching algorithm exploiting OpenStreetMap. As the GPS signal is poor in several parts of the old city the integration of the pedometer enables the navigator to obtain a sufficiently reliable position estimate, crucial for AR applications and geofencing. Within the application, there are several options given to the user to view the navigation path through the city, ranging from a satellite image of the streets to a vector map. In the navigation pane, the geofences relating to the AR experiences and other points of interest can be seen.

- Participant: Thibaud Michel
- Contact: Nabil Layaïda
- Publication: [On Mobile Augmented Reality Applications based on Geolocation](#)
- URL: <http://tyrex.inria.fr/projects/mrb.html>

## 6.4. TyrAr

*Geo Augmented Reality on a Smartphone*

**KEYWORDS:** Augmented reality - Smartphone - Geolocation

**FUNCTIONAL DESCRIPTION:** This application is an AR viewer to name the mountains, cities and historical buildings over the camera feed of the smartphone. The user can turn on himself with his device to discover names and information about Points of Interest (POIs). POIs are directly extracted from the OSM database thanks to the Overpass Turbo API. POIs are displayed on the screen with their name, an icon and an extra information. City POIs exhibit the number of inhabitants, mountains are associated to their altitude and historical buildings display their date of construction.

- Participant: Thibaud Michel
- Contact: Nabil Layaïda
- Publication: [On Mobile Augmented Reality Applications based on Geolocation](#)
- URL: <http://tyrex.inria.fr/projects/mrb.html>

## 6.5. AmiAr

*Smart Home Augmented Reality on a Smartphone*

**KEYWORDS:** Augmented reality - Smart home - Smartphone - Indoor geolocalisation

**FUNCTIONAL DESCRIPTION:** This application is a proof of concept of a Geo AR system in a smart apartment. This setup has been conducted in EquipEx Amiquel4Home. The goal here is to control objects in the apartment using widgets over the video feed from the camera. For example, a user points a lamp with his smartphone, a widget appears, then he uses a slider in this widget to modify the light intensity.

- Participant: Thibaud Michel
- Contact: Nabil Layaïda
- Publication: [On Mobile Augmented Reality Applications based on Geolocation](#)

## NON-A Project-Team

# 6. New Software and Platforms

## 6.1. Blimp

FUNCTIONAL DESCRIPTION: Scientific research and development on the control of autonomous airship have shown a significant growth in recent years. New applications appear in the areas such as freight carrier, advertising, monitoring, surveillance, transportation, military and scientific research. The control of autonomous airship is a very important problem for the aerial robots research.

The development of Blimp by Non-A is used for experimentation and demonstration of controlling algorithms. The blimp is required to provide some environment information and status of itself, such as surveillance video of surrounding environment, gesture of blimp, altitude of blimp. With these basic information, one could localize blimp with certain algorithm (visual SLAM for example) or implement one controller in order to improve the stability and maneuverability of blimp.

- Contact: Jean-Pierre Richard

## 6.2. SLIM

FUNCTIONAL DESCRIPTION: Multi-robots cooperation can be found as an application in many domains of science and technology: manufacturing, medical robotics, personal assistance, military/security and spatial robots. The market of robots is quickly developing and its capacity is continuously growing. Concerning cooperation of mobile multi-robots, 3 key issues have to be studied: Localization, path planning and robust control, for which Non-A team has worked and proposed new algorithms. Due to the ADT SLIM, we implement our algorithms (localization, path planning and robust control) and integrate them into ROS (Robotic Operating System) as a package, named SLIM.

- Contact: Jean-Pierre Richard

**QUANTIC Project-Team (section vide)**

## SPHINX Project-Team

# 6. New Software and Platforms

## 6.1. GetDDM

KEYWORDS: Large scale - 3D - Domain decomposition - Numerical solver

FUNCTIONAL DESCRIPTION: GetDDM combines GetDP and Gmsh to solve large scale finite element problems using optimized Schwarz domain decomposition methods.

- Contact: Xavier Antoine
- URL: <http://onelab.info/wiki/GetDDM>

## 6.2. GPESLab

*Gross-Pitaevskii equations Matlab toolbox*

KEYWORDS: 3D - Quantum chemistry - 2D

FUNCTIONAL DESCRIPTION: GPESLab is a Matlab toolbox developed to help physicists for computing ground states or dynamics of quantum systems modeled by Gross-Pitaevskii equations. This toolbox allows the user to define a large range of physical problems (1d-2d-3d equations, general nonlinearities, rotation term, multi-components problems...) and proposes numerical methods that are robust and efficient.

- Contact: Xavier Antoine
- URL: <http://gpelab.math.cnrs.fr/>

## **TROPICAL Team**

# 6. New Software and Platforms

## 6.1. Coq-Polyhedra

KEYWORDS: Coq - Polyhedra - Automated theorem proving - Linear optimization

SCIENTIFIC DESCRIPTION: Coq-Polyhedra is a library providing a formalization of convex polyhedra in the Coq proof assistant. While still in active development, it provides an implementation of the simplex method, and already handles the basic properties of polyhedra such as emptiness, boundedness, membership. Several fundamental results in the theory of convex polyhedra, such as Farkas Lemma, duality theorem of linear programming, and Minkowski Theorem, are also formally proved.

The formalization is based on the Mathematical Components library, and makes an extensive use of the boolean reflection methodology.

FUNCTIONAL DESCRIPTION: Coq-Polyhedra is a library which aims at formalizing convex polyhedra in Coq

- Participants: Xavier Allamigeon, Vasileios Charisopoulos and Ricardo Katz
- Partner: CIFASIS
- Contact: Xavier Allamigeon
- Publication: [A Formalization of Convex Polyhedra Based on the Simplex Method](#)
- URL: <https://github.com/nhojem/Coq-Polyhedra>

## DOLPHIN Team

## 6. New Software and Platforms

### 6.1. Grid'5000

*Grid'5000 experimental platform*

**FUNCTIONAL DESCRIPTION:** The Grid'5000 experimental platform is a scientific instrument to support computer science research related to distributed systems, including parallel processing, high performance computing, cloud computing, operating systems, peer-to-peer systems and networks. It is distributed on 10 sites in France and Luxembourg, including Lyon. Grid'5000 is a unique platform as it offers to researchers many and varied hardware resources and a complete software stack to conduct complex experiments, ensure reproducibility and ease understanding of results.

- Participants: Christian Pérez, David Loup, Frédéric Desprez, Laurent Lefèvre, Laurent Pouilloux, Marc Pinède and Simon Delamare
- Contact: Frédéric Desprez
- URL: <https://www.grid5000.fr/mediawiki/index.php/Grid5000:Home>

### 6.2. ParadisEO

**KEYWORD:** Parallelisation

**SCIENTIFIC DESCRIPTION:** ParadisEO (PARallel and DIStributed Evolving Objects) is a C++ white-box object-oriented framework dedicated to the flexible design of metaheuristics. Based on EO, a template-based ANSI-C++ compliant evolutionary computation library, it is composed of four modules: \* Paradiseo-EO provides tools for the development of population-based metaheuristic (Genetic algorithm, Genetic programming, Particle Swarm Optimization (PSO)...) \* Paradiseo-MO provides tools for the development of single solution-based metaheuristics (Hill-Climbing, Tabu Search, Simulated annealing, Iterative Local Search (ILS), Incremental evaluation, partial neighborhood...) \* Paradiseo-MOEO provides tools for the design of Multi-objective metaheuristics (MO fitness assignment schemes, MO diversity assignment schemes, Elitism, Performance metrics, Easy-to-use standard evolutionary algorithms...) \* Paradiseo-PEO provides tools for the design of parallel and distributed metaheuristics (Parallel evaluation, Parallel evaluation function, Island model) Furthermore, ParadisEO also introduces tools for the design of distributed, hybrid and cooperative models: \* High level hybrid metaheuristics: coevolutionary and relay model \* Low level hybrid metaheuristics: coevolutionary and relay model

**FUNCTIONAL DESCRIPTION:** Paradiseo is a software framework for metaheuristics (optimisation algorithms aimed at solving difficult optimisation problems). It facilitates the use, development and comparison of classic, multi-objective, parallel or hybrid metaheuristics.

- Partners: CNRS - Université Lille 1
- Contact: El-Ghazali Talbi
- URL: <http://paradiseo.gforge.inria.fr/>

### 6.3. VRPsolve

**KEYWORDS:** C++ - Mobile Computing, Transportation - Optimization

SCIENTIFIC DESCRIPTION: VRPsolve is a software for solving vehicle routing problems dealing with last-mile delivery issues that arise as we approach the final customer. When modeling and solving combinatorial optimization problems, especially problems related to the transport of goods and people, the resulting models are generally subject to a specific development in order to be validated, as industrial needs are highly dependent of the application domain. However, a set of conventional objectives and constraints, such as vehicles capacities, incompatible parcels, time windows, are now commonly encountered. In addition to being efficient and effective, VRPsolve differentiates from other tools by allowing to quickly and conveniently integrate ad-hoc constraints and objectives into a generic software. Indeed, VRPsolve effectively deal with industrial last-mile delivery vehicle routing problems and is able to cope with multiple objectives and a large number of constraints by using advanced optimization algorithms which are usually not available with existing softwares. In addition, VRPsolve allows industrial collaborations to be addressed by solving real-world problems requiring geographic information systems (GIS).

- Participants: Arnaud Liefoghe, Clive Ferret-Canape and Sébastien Vérel
- Contact: Clive Ferret-Canape
- URL: <http://gforge.inria.fr/projects/vrpsolve>

## 6.4. Platform Grid'5000

The Dolphin project-team has been the Principal Investigator of the Grid5000@Lille project funded (budget: 750K€) within the framework of the CPER. This project consists in building in 2017 a new site of the Grid'5000 platform at Lille. This new site hosted by Inria Lille replaces the old one which was located in the supercomputing center (CRI) of the University of Lille. It consists in a GPU-enhanced computing cluster composed of over 1.000 CPU cores and 60.000 GPU cores corresponding to a 20FLOPS computational power. The Grid5000@Lille project allowed also the recruitment of two engineers for the system and network administration and the software development for two years. Another upgrade with more GPUs is planned for the beginning of 2018.

- Participants: F. Desprez, F. Huet, E. Jeannot, Y. Jegou, A. Lebre, L. Lefevre, F. Loui, D. Margery, N. Melab, J-M. Menaud, P. Neyron, L. Nussbaum, C. Perez, J-M. Pierson, O. Richard., S. Varette.
- Contact: Nouredine Melab
- URL: <https://www.grid5000.fr/mediawiki/index.php/Grid5000:Home>

## GEOSTAT Project-Team

# 6. New Software and Platforms

## 6.1. Fluex

KEYWORDS: Signal - Signal processing

SCIENTIFIC DESCRIPTION: Fluex is a package consisting of the Microcanonical Multiscale Formalism for 1D, 2D 3D and 3D+t general signals.

FUNCTIONAL DESCRIPTION: Fluex is a C++ library developed under Gforge. Fluex is a library in nonlinear signal processing. Fluex is able to analyze turbulent and natural complex signals, Fluex is able to determine low level features in these signals that cannot be determined using standard linear techniques.

- Participants: Hussein Yahia and Rémi Paties
- Contact: Hussein Yahia
- URL: <http://fluex.gforge.inria.fr/>

## 6.2. FluidExponents

KEYWORDS: Signal processing - Wavelets - Fractal - Spectral method - Complexity

FUNCTIONAL DESCRIPTION: FluidExponents is a signal processing software dedicated to the analysis of complex signals displaying multiscale properties. It analyzes complex natural signals by use of nonlinear methods. It implements the multifractal formalism and allows various kinds of signal decomposition and reconstruction. One key aspect of the software lies in its ability to evaluate key concepts such as the degree of unpredictability around a point in a signal, and provides different kinds of applications. The software can be used for times series or multidimensional signals.

- Participants: Antonio Turiel and Hussein Yahia
- Contact: Hussein Yahia
- URL: <https://fluidexponents@scm.gforge.inria.fr/svn/fluidexponents/FluidExponents>

## 6.3. classifemo

KEYWORDS: Classification - Audio

FUNCTIONAL DESCRIPTION: Classifies vocal audio signals. Classifemo extracts characteristics from vocal audio signals. These characteristics are extracted from signals of different type: initially these were emotion databases, but it can also process signals recorded from patients with motor speech disorders. The software can train usual classifiers (SVM, random forests, etc) on these databases as well as classify new signals.

- Participants: Khalid Daoudi and Nicolas Brodu
- Contact: Khalid Daoudi
- URL: <https://allgo.inria.fr/app/emotionclassifierprototype>

## 6.4. superres

*Super-Resolution of multi-spectral and multi-resolution images*

KEYWORD: Multiscale

SCIENTIFIC DESCRIPTION: This resolution enhancement method is designed for multispectral and multiresolution images, such as these provided by the Sentinel-2 satellites (but not only). Starting from the highest resolution bands, band-dependent information (reflectance) is separated from information that is common to all bands (geometry of scene elements). This model is then applied to unmix low-resolution bands, preserving their reflectance, while propagating band-independent information to preserve the sub-pixel details.

FUNCTIONAL DESCRIPTION: This super-resolution software for multi-spectral images consists of: - A core C++ library, which can be used directly - A Python module interface to this library - A Java JNI interface to the library - An end-user Python script for super-resolving Sentinel-2 images - An end-user plugin for the widely used SNAP software of the ESA.

- Participant: Nicolas Brodu
- Contact: Nicolas Brodu
- URL: <http://nicolas.brodu.net/recherche/superres/index.html>

## 6.5. EdgeReconstruct

*Edge Reconstruction With UPM Manifold*

KEYWORDS: 2D - Fractal - Signal processing

FUNCTIONAL DESCRIPTION: EdgeReconstruct is a software that reconstructs a complex signal from the computation of most unpredictable points in the framework of the Microcanonical Multifractal Formalism. The quality of the reconstruction is also evaluated. The software is a companion of a paper published in 2013: <https://hal.inria.fr/hal-00924137>.

- Contact: Suman Kumar Maji
- URL: <https://geostat.bordeaux.inria.fr/index.php/downloads.html>

## INOCS Team

## 6. New Software and Platforms

### 6.1. dapcstp

*A dual-ascent-based branch-and-bound framework for the prize-collecting Steiner tree and related problems*

KEYWORDS: Mathematical Optimization - Systems Biology

FUNCTIONAL DESCRIPTION: Variants of the Steiner tree problem appear in a broad range of diverse applications, ranging from infrastructure network design to the analysis of biological networks and pattern recognition. In this software, we provide a branch-and-bound (B&B) framework for solving the asymmetric prize-collecting Steiner tree problem (APCSTP). Several well-known network design problems can be transformed to the APCSTP, including the Steiner tree problem (STP), prize-collecting Steiner tree problem (PCSTP), maximum-weight connected subgraph problem (MWCS) and the node-weighted Steiner tree problem (NW-STP).

- Contact: Markus Sinnl
- URL: <https://github.com/mluipersbeck/dapcstp>

### 6.2. HappyChic-ApproPick

KEYWORDS: Operational research - Optimization - Java

FUNCTIONAL DESCRIPTION: This software is a prototype developed for the bilateral contract with the company HappyChic. This software is a solver for an integrated warehouse order picking problem with manual picking operations. More precisely, the following problems are solved: (1) the assignment of references to storage positions, based on the iterative solving of minimum cost flow problems, (2) the division of clients orders into several parcels, respecting weight and size constraints, using a dynamic programming algorithm based on the split algorithm, (3) the batching of parcels into trolleys to perform picking tours, using a dynamic programming algorithm based on the split algorithm. The objective function is to minimize the total walking distance. This software is designed to deal with the large-sized industrial instances of HappyChic (considering hundreds of clients, thousands of positions and product references) in a short computation time (few minutes).

- Contact: Maxime Ogier

### 6.3. rcmwcs

*A Relax-and-Cut Algorithm for Maximum Weight Connected Subgraph Problems*

KEYWORDS: Mathematical Optimization - Systems Biology

FUNCTIONAL DESCRIPTION: Finding maximum weight connected subgraphs within networks is a fundamental combinatorial optimization problem both from a theoretical and a practical standpoint. One of the most prominent applications of this problem appears in Systems Biology and it corresponds to the detection of active subnetworks within gene interaction networks. The software is a framework to solve the model by means of Relax-and-Cut, i.e., Lagrangian relaxation combined with constraint generation.

- Contact: Markus Sinnl
- URL: <https://msinnl.github.io/pages/rcmwcs.html>

### 6.4. MIBLPsolver

*A Solver for Mixed-Integer Bilevel Linear Problems*

KEYWORD: Mathematical Optimization

**FUNCTIONAL DESCRIPTION:** Bilevel optimization problems are very challenging optimization models arising in many important practical contexts, including pricing mechanisms in the energy sector, airline and telecommunication industry, transportation networks, optimal expansion of gas networks, critical infrastructure defense, and machine learning. In this software, we present a new general purpose branch-and-cut framework for the exact solution of mixed-integer bilevel linear programs (MIBLP), which constitute a very significant subfamily of bilevel optimization problems.

- Contact: Markus Sinnl
- URL: <https://msinnl.github.io/pages/bilevel.html>

## 6.5. PARROT

*Planning Adapter Performing ReRouting and Optimization of Timing*

**KEYWORDS:** Decision aid - Railway - Scheduling

**FUNCTIONAL DESCRIPTION:** This is a decision support system addressing the problem of the rescheduling railway schedules on the Belgian network when maintenance operations are planned in the short term (2-3 weeks in advance). The deliverable is a software tool that will take as input: (1) the schedules initially planned for the different trains, (2) the initial routes of the trains, (3) maintenance operations / changes of elements in the form of constraints (unavailable routes etc.). He then provides in output: (1) the new train schedule, (2) the new routing of the fleet. The modifications must respect the constraints corresponding to the operations of maintenance. For example, in some cases it is common to leave at least a few minutes interval between two trains using the same track in the station. This constraint must then be propagated if a maintenance operation delays the arrival of a train. New schedules and routings have to be created following a specific goal. Changes made to schedules and routings must minimize: (1) variations on the time spent at the station, (2) the number of partially canceled trains (additional correspondence (s) or stations that are no longer served), (2) the number of fully canceled trains (no stations served).

- Contact: Martine Labbe

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## MISTIS Project-Team

## 6. New Software and Platforms

### 6.1. BOLD model FIT

KEYWORDS: Functional imaging - FMRI - Health

FUNCTIONAL DESCRIPTION: This Matlab toolbox performs the automatic estimation of biophysical parameters using the extended Balloon model and BOLD fMRI data. It takes as input a MAT file and provides as output the parameter estimates achieved by using stochastic optimization

- Authors: Jan M Warnking, Pablo Mesejo Santiago and Florence Forbes
- Contact: Pablo Mesejo Santiago
- URL: <https://hal.archives-ouvertes.fr/hal-01221115v2/>

### 6.2. MMST

*Mixtures of Multiple Scaled Student T distributions*

KEYWORDS: Medical imaging - Brain MRI - Statistics - Health - Robust clustering

FUNCTIONAL DESCRIPTION: The package implements mixtures of so-called multiple scaled Student distributions, which are generalisation of multivariate Student T distribution allowing different tails in each dimension. Typical applications include Robust clustering to analyse data with possible outliers. In this context, the model and package have been used on large data sets of brain MRI to segment and identify brain tumors.

- Participants: Alexis Arnaud, Darren Wraith and Florence Forbes
- Contact: Florence Forbes
- URL: <http://mistis.inrialpes.fr/realisations.html>

### 6.3. PyHRF

KEYWORDS: Health - Brain - IRM - Neurosciences - Statistic analysis - FMRI - Medical imaging

FUNCTIONAL DESCRIPTION: As part of fMRI data analysis, PyHRF provides a set of tools for addressing the two main issues involved in intra-subject fMRI data analysis : (i) the localization of cerebral regions that elicit evoked activity and (ii) the estimation of the activation dynamics also referenced to as the recovery of the Hemodynamic Response Function (HRF). To tackle these two problems, PyHRF implements the Joint Detection-Estimation framework (JDE) which recovers parcel-level HRFs and embeds an adaptive spatio-temporal regularization scheme of activation maps.

- Participants: Aina Frau Pascual, Christine Bakhous, Florence Forbes, Jaime Eduardo Arias Almeida, Laurent Risser, Lotfi Chaari, Philippe Ciuciu, Solveig Badillo, Thomas Perret and Thomas Vincent
- Partners: CEA - NeuroSpin
- Contact: Florence Forbes
- URL: <http://pyhrf.org>

### 6.4. xLLiM

*High dimensional locally linear mapping*

KEYWORDS: Clustering - Regression

FUNCTIONAL DESCRIPTION: This is an R package available on the CRAN at <https://cran.r-project.org/web/packages/xLLiM/index.html>

xLLiM provides a tool for non linear mapping (non linear regression) using a mixture of regression model and an inverse regression strategy. The methods include the GLLiM model (Deleforge et al (2015) ) based on Gaussian mixtures and a robust version of GLLiM, named SLLiM (see Perthame et al (2016) ) based on a mixture of Generalized Student distributions.

- Participants: Antoine Deleforge, Emeline Perthame and Florence Forbes
- Contact: Florence Forbes
- URL: <https://cran.r-project.org/web/packages/xLLiM/index.html>

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## MODAL Project-Team

## 6. New Software and Platforms

### 6.1. MixtComp

#### *Mixture Computation*

KEYWORDS: Clustering - Statistics - Missing data

FUNCTIONAL DESCRIPTION: MixtComp (Mixture Computation) is a model-based clustering package for mixed data originating from the Modal team (Inria Lille). It has been engineered around the idea of easy and quick integration of all new univariate models, under the conditional independence assumption. New models will eventually be available from researches, carried out by the Modal team or by other teams. Currently, central architecture of MixtComp is built and functionality has been field-tested through industry partnerships. Three basic models (Gaussian, multinomial, Poisson) are implemented, as well as two advanced models (Ordinal and Rank). MixtComp has the ability to natively manage missing data (completely or by interval). MixtComp is used as an R package, but its internals are coded in C++ using state of the art libraries for faster computation.

- Participants: Christophe Biernacki, Étienne Goffinet, Matthieu Marbac-Lourdelle, Quentin Grimonprez, Serge Iovleff and Vincent Kubicki
- Contact: Christophe Biernacki
- URL: <https://modal-research.lille.inria.fr/BigStat>

### 6.2. BlockCluster

#### *Block Clustering*

KEYWORDS: Statistic analysis - Clustering package

SCIENTIFIC DESCRIPTION: Simultaneous clustering of rows and columns, usually designated by biclustering, co-clustering or block clustering, is an important technique in two way data analysis. It consists of estimating a mixture model which takes into account the block clustering problem on both the individual and variables sets. The blockcluster package provides a bridge between the C++ core library and the R statistical computing environment. This package allows to co-cluster binary, contingency, continuous and categorical data-sets. It also provides utility functions to visualize the results. This package may be useful for various applications in fields of Data mining, Information retrieval, Biology, computer vision and many more.

FUNCTIONAL DESCRIPTION: BlockCluster is an R package for co-clustering of binary, contingency and continuous data based on mixture models.

- Participants: Christophe Biernacki, Gilles Celeux, Parmeet Bhatia, Serge Iovleff, Vincent Brault and Vincent Kubicki
- Partner: Université de Technologie de Compiègne
- Contact: Serge Iovleff
- URL: <http://cran.r-project.org/web/packages/blockcluster/index.html>

### 6.3. CloHe

#### *Clustering of Mixed data*

KEYWORDS: Classification - Clustering - Missing data

FUNCTIONAL DESCRIPTION: Software of classification for mixed data with missing values with application to multispectral satellite image time-series

- Partners: CNRS - INRA
- Contact: Serge Iovleff
- URL: <https://modal.lille.inria.fr/CloHe/>

## 6.4. PACBayesianNMF

KEYWORDS: Statistics - Machine learning

FUNCTIONAL DESCRIPTION: Implementing NMF with a PAC-Bayesian approach relying upon block gradient descent

- Participants: Benjamin Guedj and Astha Gupta
- Contact: Benjamin Guedj
- URL: <https://github.com/astha736/PACbayesianNMF>

## 6.5. pycobra

KEYWORDS: Statistics - Data visualization - Machine learning

SCIENTIFIC DESCRIPTION: pycobra is a python library for ensemble learning, which serves as a toolkit for regression, classification, and visualisation. It is scikit-learn compatible and fits into the existing scikit-learn ecosystem.

pycobra offers a python implementation of the COBRA algorithm introduced by Biau et al. (2016) for regression.

Another algorithm implemented is the EWA (Exponentially Weighted Aggregate) aggregation technique (among several other references, you can check the paper by Dalalyan and Tsybakov (2007)).

Apart from these two regression aggregation algorithms, pycobra implements a version of COBRA for classification. This procedure has been introduced by Mojirsheibani (1999).

pycobra also offers various visualisation and diagnostic methods built on top of matplotlib which lets the user analyse and compare different regression machines with COBRA. The Visualisation class also lets you use some of the tools (such as Voronoi Tessellations) on other visualisation problems, such as clustering.

- Participants: Bhargav Srinivasa Desikan and Benjamin Guedj
- Contact: Benjamin Guedj
- URL: <https://github.com/bhargavvader/pycobra>

## 6.6. STK++

*Statistical ToolKit*

KEYWORDS: Statistics - Linear algebra - Framework - Learning - Statistical learning

FUNCTIONAL DESCRIPTION: STK++ (Statistical ToolKit in C++) is a versatile, fast, reliable and elegant collection of C++ classes for statistics, clustering, linear algebra, arrays (with an API Eigen-like), regression, dimension reduction, etc. The library is interfaced with lapack for many linear algebra usual methods. Some functionalities provided by the library are available in the R environment using rtkpp and rtkore.

STK++ is suitable for projects ranging from small one-off projects to complete data mining application suites.

- Participant: Serge Iovleff
- Contact: Serge Iovleff
- URL: <http://www.stkpp.org>

## 6.7. rtkore

*STK++ core library integration to R using Rcpp*

KEYWORDS: C++ - Data mining - Clustering - Statistics - Regression

FUNCTIONAL DESCRIPTION: STK++ (<http://www.stkpp.org>) is a collection of C++ classes for statistics, clustering, linear algebra, arrays (with an Eigen-like API), regression, dimension reduction, etc. The integration of the library to R is using Rcpp. The rtkore package includes the header files from the STK++ core library. All files contain only templated classes or inlined functions. STK++ is licensed under the GNU LGPL version 2 or later. rtkore (the stkpp integration into R) is licensed under the GNU GPL version 2 or later. See file LICENSE.note for details.

- Participant: Serge Iovleff
- Contact: Serge Iovleff
- URL: <https://cran.r-project.org/web/packages/rtkore/index.html>

## 6.8. Platforms

### 6.8.1. MASSICCC Platform

MASSICCC is a demonstration platform giving access through a SaaS (service as a software) concept to data analysis libraries developed at Inria. It allows to obtain results either directly through a website specific display (specific and interactive visual outputs) or through an R data object download. It started in October 2015 for two years and is common to the Modal team (Inria Lille) and the Select team (Inria Saclay). In 2016, two packages have been integrated: Mixmod and MixtComp (see the specific section about MixtComp). In 2017, the BlockCluster package has been integrated and also a particular attention to provide meaningful graphical outputs (for Mixmod, MixtComp and BlockCluster) directly in the web platform itself has led to some specific developments.

**RANDOPT Team (section vide)**

## REALOPT Project-Team

## 6. New Software and Platforms

### 6.1. BaPCod

*A generic Branch-And-Price-And-Cut Code*

KEYWORDS: Column Generation - Branch-and-Price - Branch-and-Cut - Mixed Integer Programming - Mathematical Optimization - Benders Decomposition - Dantzig-Wolfe Decomposition - Extended Formulation

FUNCTIONAL DESCRIPTION: BaPCod is a prototype code that solves Mixed Integer Programs (MIP) by application of reformulation and decomposition techniques. The reformulated problem is solved using a branch-and-price-and-cut (column generation) algorithms, Benders approaches, network flow and dynamic programming algorithms. These methods can be combined in several hybrid algorithms to produce exact or approximate solutions (primal solutions with a bound on the deviation to the optimum).

- Participants: Artur Alves Pessoa, Boris Detienne, Eduardo Uchoa Barboza, Franck Labat, François Clautiaux, François Vanderbeck, Halil Sen, Issam Tahiri, Michael Poss, Pierre Pesneau, Romain Leguay and Ruslan Sadykov
- Partners: Université de Bordeaux - CNRS - IPB - Universidade Federal Fluminense
- Contact: François Vanderbeck
- URL: <https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod>

### 6.2. WineryPlanning

- Participants: Agnes Le Roux, Alexis Toullat, François Vanderbeck, Issam Tahiri and Ruslan Sadykov
- Contact: François Vanderbeck

### 6.3. ORTOJ

*Operation Research Tools Under Julia*

KEYWORDS: Modeling - Processing - Dashboard

FUNCTIONAL DESCRIPTION: This set of tools currently includes : 1) BlockJuMP.jl: extension of JuMP to model decomposable mathematical programs (using either Benders or Dantzig-Wolfe decomposition paradigm) 2) Scanner.jl: a default data parser to ease the reading of the input data in the form that they are often encountered in operational research. 3) BenchmarkUtils.jl: Tools to ease the setup of numerical experiments to benchmark algorithmic feature performances. The test automation permits to quickly calibrate the parameters of an arbitrary algorithm control function.

- Participants: François Vanderbeck, Guillaume Marques, Issam Tahiri and Ruslan Sadykov
- Contact: Issam Tahiri

## SELECT Project-Team

# 5. New Software and Platforms

## 5.1. BlockCluster

### *Block Clustering*

KEYWORDS: Statistic analysis - Clustering package

SCIENTIFIC DESCRIPTION: Simultaneous clustering of rows and columns, usually designated by biclustering, co-clustering or block clustering, is an important technique in two way data analysis. It consists of estimating a mixture model which takes into account the block clustering problem on both the individual and variables sets. The blockcluster package provides a bridge between the C++ core library and the R statistical computing environment. This package allows to co-cluster binary, contingency, continuous and categorical data-sets. It also provides utility functions to visualize the results. This package may be useful for various applications in fields of Data mining, Information retrieval, Biology, computer vision and many more.

FUNCTIONAL DESCRIPTION: BlockCluster is an R package for co-clustering of binary, contingency and continuous data based on mixture models.

- Participants: Christophe Biernacki, Gilles Celeux, Parmeet Bhatia, Serge Iovleff, Vincent Brault and Vincent Kubicki
- Partner: Université de Technologie de Compiègne
- Contact: Serge Iovleff
- URL: <http://cran.r-project.org/web/packages/blockcluster/index.html>

## 5.2. MASSICCC

### *Massive Clustering with Cloud Computing*

KEYWORDS: Statistic analysis - Big data - Machine learning - Web Application

SCIENTIFIC DESCRIPTION: The web application let users use several software packages developed by Inria directly in a web browser. Mixmod is a classification library for continuous and categorical data. MixtComp allows for missing data and a larger choice of data types. BlockCluster is a library for co-clustering of data. When using the web application, the user can first upload a data set, then configure a job using one of the libraries mentioned and start the execution of the job on a cluster. The results are then displayed directly in the browser allowing for rapid understanding and interactive visualisation.

FUNCTIONAL DESCRIPTION: The MASSICCC web application offers a simple and dynamic interface for analysing heterogeneous data with a web browser. Various software packages for statistical analysis are available (Mixmod, MixtComp, BlockCluster) which allow for supervised and supervised classification of large data sets.

- Contact: Jonas Renault
- URL: <https://massiccc.lille.inria.fr>

## 5.3. Mixmod

### *Many-purpose software for data mining and statistical learning*

KEYWORDS: Data modeling - Mixed data - Classification - Data mining - Big data

FUNCTIONAL DESCRIPTION: Mixmod is a free toolbox for data mining and statistical learning designed for large and highdimensional data sets. Mixmod provides reliable estimation algorithms and relevant model selection criteria.

It has been successfully applied to marketing, credit scoring, epidemiology, genomics and reliability among other domains. Its particularity is to propose a model-based approach leading to a lot of methods for classification and clustering.

Mixmod allows to assess the stability of the results with simple and thorough scores. It provides an easy-to-use graphical user interface (mixmodGUI) and functions for the R (Rmixmod) and Matlab (mixmodForMatlab) environments.

- Participants: Benjamin Auder, Christophe Biernacki, Florent Langrognnet, Gérard Govaert, Gilles Celeux, Remi Lebrete and Serge Iovleff
- Partners: CNRS - Université Lille 1 - LIFL - Laboratoire Paul Painlevé - HEUDIASYC - LMB
- Contact: Gilles Celeux
- URL: <http://www.mixmod.org>

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## SEQUEL Project-Team

## 6. New Software and Platforms

### 6.1. BAC

*Bayesian Policy Gradient and Actor-Critic Algorithms*

KEYWORDS: Machine learning - Incremental learning - Policy Learning

FUNCTIONAL DESCRIPTION: To address this issue, we proceed to supplement our Bayesian policy gradient framework with a new actor-critic learning model in which a Bayesian class of non-parametric critics, based on Gaussian process temporal difference learning, is used. Such critics model the action-value function as a Gaussian process, allowing Bayes' rule to be used in computing the posterior distribution over action-value functions, conditioned on the observed data. Appropriate choices of the policy parameterization and of the prior covariance (kernel) between action-values allow us to obtain closed-form expressions for the posterior distribution of the gradient of the expected return with respect to the policy parameters. We perform detailed experimental comparisons of the proposed Bayesian policy gradient and actor-critic algorithms with classic Monte-Carlo based policy gradient methods, as well as with each other, on a number of reinforcement learning problems.

- Contact: Michal Valko
- URL: <https://team.inria.fr/sequel/Software/BAC/>

### 6.2. GuessWhat?!

*GuessWhat?! Visual object discovery through multi-modal dialogue*

KEYWORDS: Deep learning - Dialogue System

FUNCTIONAL DESCRIPTION: This project train a AI to play the GuessWhat?! game. Thus, you can train an AI to ask questions, to answer questions about images. You can also perform basic visual reasoning. This project is a testbed for future interactive dialogue system.

- Partner: Universite de Montreal
- Contact: Florian Strub
- Publications: [GuessWhat?! Visual object discovery through multi-modal dialogue - End-to-end optimization of goal-driven and visually grounded dialogue systems Harm de Vries](#)

### 6.3. Squeak

*Sequential sampling for kernel matrix approximation*

KEYWORD: Machine learning

- Contact: Daniele Calandriello
- URL: <http://researchers.lille.inria.fr/~valko/hp/serve.php?what=publications/squeak.py>

### 6.4. OOR

*Optimistic Optimization in R*

KEYWORDS: Black-box optimization - Machine learning

- Contact: Mickael Binois
- URL: <https://cran.r-project.org/web/packages/OOR/index.html>

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## SIERRA Project-Team

# 5. New Software and Platforms

## 5.1. ProxASAGA

KEYWORD: Optimization

FUNCTIONAL DESCRIPTION: A C++/Python code implementing the methods in the paper "Breaking the Nonsmooth Barrier: A Scalable Parallel Method for Composite Optimization", F. Pedregosa, R. Leblond and S. Lacoste-Julien, Advances in Neural Information Processing Systems (NIPS) 2017. Due to their simplicity and excellent performance, parallel asynchronous variants of stochastic gradient descent have become popular methods to solve a wide range of large-scale optimization problems on multi-core architectures. Yet, despite their practical success, support for nonsmooth objectives is still lacking, making them unsuitable for many problems of interest in machine learning, such as the Lasso, group Lasso or empirical risk minimization with convex constraints. In this work, we propose and analyze ProxASAGA, a fully asynchronous sparse method inspired by SAGA, a variance reduced incremental gradient algorithm. The proposed method is easy to implement and significantly outperforms the state of the art on several nonsmooth, large-scale problems. We prove that our method achieves a theoretical linear speedup with respect to the sequential version under assumptions on the sparsity of gradients and block-separability of the proximal term. Empirical benchmarks on a multi-core architecture illustrate practical speedups of up to 12x on a 20-core machine.

- Contact: Fabian Pedregosa
- URL: <https://github.com/fabianp/ProxASAGA>

## 5.2. object-states-action

KEYWORD: Computer vision

FUNCTIONAL DESCRIPTION: Code for the paper Joint Discovery of Object States and Manipulation Actions, ICCV 2017: Many human activities involve object manipulations aiming to modify the object state. Examples of common state changes include full/empty bottle, open/closed door, and attached/detached car wheel. In this work, we seek to automatically discover the states of objects and the associated manipulation actions. Given a set of videos for a particular task, we propose a joint model that learns to identify object states and to localize state-modifying actions. Our model is formulated as a discriminative clustering cost with constraints. We assume a consistent temporal order for the changes in object states and manipulation actions, and introduce new optimization techniques to learn model parameters without additional supervision. We demonstrate successful discovery of seven manipulation actions and corresponding object states on a new dataset of videos depicting real-life object manipulations. We show that our joint formulation results in an improvement of object state discovery by action recognition and vice versa.

- Contact: Jean-Baptiste Alayrac

## TAU Team

## 6. New Software and Platforms

### 6.1. io.datascience

#### *Input Output Data Science*

KEYWORDS: Open data - Semantic Web - FAIR (Findable, Accessible, Interoperable, and Reusable)

FUNCTIONAL DESCRIPTION: io.datascience (Input Output Data Science) is the instance of the Linked Wiki platform developed specifically in Paris-Saclay University as part of its Center for Data Science.

The goal of io.datascience: to facilitate the sharing and use of scientific data. The technological concept of io.datascience: the exploitation of semantic web advances, and in particular wiki technologies.

One of the grand challenges of data-intensive science is to facilitate knowledge discovery by assisting humans and machines in their discovery of, access to, integration and analysis of, task-appropriate scientific data and their associated algorithms and workflows. The guiding principles for this challenge have been defined: Data should become FAIR (Findable, Accessible, Interoperable, and Reusable) (Wilkinson, M., and The FAIR Guiding Principles for Scientific Data Management and Stewardship, Nature Scientific Data 2016)

io.datascience is both a data sharing platform and a framework for further development. It realizes a practical implementation of FAIR principles through a user-centric approach. • Share: Software users can declare the sources of the data they use as well as their query requests. • Discover: Using a form, users can link their data sources to each other. The repository used is that of Wikidata. The user can then retrieve his data sources and example queries through a search interface or directly through Google and Wikipedia. • Reuse: data is identified and qualified, a simple interface allows the user to provide the desired level of description for the data they refer to, as well as examples of use. • Analyze: io.datascience will soon be proposing the creation of RDF databases on the cloud on the cloud of Paris Sud University.

- Partners: Border Cloud - Paris Saclay Center for Data Science - Université Paris-Sud
- Contact: Cécile Germain-Renaud
- Publications: [Data acquisition for analytical platforms: Automating scientific workflows and building an open database platform for chemical analysis metadata](#) - [A platform for scientific data sharing](#) - [TFT, Tests For Triplestores](#) - [Une autocomplétion générique de SPARQL dans un contexte multi-services](#) - [Certifying the interoperability of RDF database systems](#) - [Transforming Wikipedia into an Ontology-based Information Retrieval Search Engine for Local Experts using a Third-Party Taxonomy](#) - [The Grid Observatory 3.0](#) - [Towards reproducible research and open collaborations using semantic technologies](#)
- URL: <https://io.datascience-paris-saclay.fr/>

### 6.2. Codalab

KEYWORDS: Benchmarking - Competition

FUNCTIONAL DESCRIPTION: Challenges in machine learning and data science are competitions running over several weeks or months to resolve problems using provided datasets or simulated environments. Challenges can be thought of as crowdsourcing, benchmarking, and communication tools. They have been used for decades to test and compare competing solutions in machine learning in a fair and controlled way, to eliminate "inventor-evaluator" bias, and to stimulate the scientific community while promoting reproducible science. See [our slide presentation](#).

As of december 2017 there are 145 public competitions on Codalab and over 10000 users. Some of the areas in which Codalab is used include Computer vision and medical image analysis, natural language processing, time series prediction, causality, and automatic machine learning. Codalab was selected for the million Euro challenge See.4C that was awarded a H2020 EU grant for its organization.

TAU is going to continue expanding Codalab to accommodate new needs. One of our current focus is to support use of challenges for teaching (i.e. include a grading system as part of Codalab) and support for hooking up data simulation engines in the backend of Codalab to enable Reinforcement Learning challenges and simulate interactions of machines with an environment. For the third year, **we are using Codalab for student projects**. M2 AIC students create mini data science challenges in teams of 6 students. L2 math and informatics students then solve them as part of their mini projects. We are collaborating with RPI (New York, USA) to use this platform as part of a curriculum of medical students. Our PhD. students are involved in co-organizing challenges to expose the research community at large with the topic of their PhD. This helps them formalizing a task with rigor and allows them to disseminate their research.

- Partner: Microsoft
- Contact: Isabelle Guyon
- URL: <http://competitions.codalab.org>

### 6.3. Cartolabe

KEYWORD: Information visualization

FUNCTIONAL DESCRIPTION: The goal of Cartolabe is to build a visual map representing the scientific activity of an institution/university/domain from published articles and reports. Using the HAL Database and building upon the AnHALytics processing chain, Cartolabe provides the user with a map of the thematics, authors and articles and their dynamics along time. ML techniques are used for dimensionality reduction, cluster and topics identification, visualisation techniques are used for a scalable 2D representation of the results.

NEWS OF THE YEAR: Improvement of the graphical interface

- Contact: Philippe Caillou
- URL: <http://cartolabe.lri.fr/>

**ASPI Team (section vide)**

## CQFD Project-Team

# 6. New Software and Platforms

## 6.1. biips

*Bayesian Inference with Interacting Particle Systems*

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

- Participants: Adrien Todeschini and François Caron
- Contact: Adrien Todeschini
- URL: <http://biips.gforge.inria.fr>

## 6.2. PCAmixdata

KEYWORD: Statistic analysis

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

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

## 6.3. QuantifQuantile

KEYWORD: Regression

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

- Contact: Jérôme Saracco

## MATHRISK Project-Team

## 5. New Software and Platforms

### 5.1. PREMIA

**KEYWORDS:** Financial products - Computational finance - Option pricing

**SCIENTIFIC DESCRIPTION:** 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 and 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.

**FUNCTIONAL DESCRIPTION:** Premia is a software designed for option pricing, hedging and financial model calibration.

- Participants: Agnes Sulem, Antonino Zanette, Aurélien Alfonsi, Benjamin Jourdain, Jacques Printems and Jérôme Lelong
- Partners: Inria - Ecole des Ponts ParisTech - Université Paris-Est
- Contact: Agnes Sulem
- URL: <http://www.premia.fr>

### 5.2. Platforms

#### 5.2.1. Development of the quantitative platform Premia in 2017

- Premia 18 has been registered at the Agence pour la Protection des Programmes APP (IDDN.FR.001.190010.014.S.C.2001.000.31000)

- Premia 19 has been delivered to the Consortium Premia on March 16th. It contains the following new algorithms : Risk Management, Model Risk, Insurance

- XVA simulation on GPUs using Nested Monte Carlo. L. Abbas Turki
- Model-independent bounds for option prices a mass transport approach. M. Beiglböck, P. H. Labordère, F. Penkner  
*Finance Stochastics Volume 17, 2013.*
- Model-Independent Pricing of Asian Options via Optimal Martingale. F Stebegg
- Pricing and Hedging GMWB in the Heston and in the Black-Scholes with Stochastic Interest Rate Models. L. Goudenege, A. Molent, A. Zanette

Equity Derivatives

- Quantization meets Fourier: a new technology for pricing options. G. Callegaro, L. Fiorin, M. Grasselli.
- Efficient unbiased simulation scheme for the SABR stochastic volatility model. B. Chen, C.W. Oosterlee J.A.M van der Weide.

*International Journal of Theoretical and Applied Finance. Vol. 15, No. 2 (2012)*

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*The Journal of Computational Finance. Vol. 16, Issue 4, 2013.*
- The evaluation of barrier option prices under stochastic volatility. C.Chiarella, B.Kang, G.H.Meyer  
*Computers and Mathematics with Applications 64, 2012.*
- Path-Dependent Volatility. J.Guyon  
*Risk Magazine, October 2014.*
- Cross-Dependent Volatility. J.Guyon  
*Risk Magazine, March 2016*
- Option pricing and implied volatilities in a 2-hypergeometric stochastic volatility model. N. Privault  
Q. She  
*Applied Mathematics Letters, 53, 2016*
- Option price with stochastic volatility for both fast and slow mean-reverting regimes. Q. Zhang, J. Han, and M. Gao.  
*C. R. Math. Acad. Sci. Paris, 351(9-10), 2013.*
- Application of the improved fast Gauss transform to option pricing under jump-diffusion processes. T. Sakuma and Y. Yamada  
*The Journal of Computational Finance, Volume 18, Issue 2, 2014.*
- Features of the Russian derivatives market volatility index development taking into account possible price jumps. A. Grechko, O. Kudryavtsev  
*Theory of Probability and Its Applications-SIAM, 2017 61:3 (2017), to appear*
- On the application of spectral filters in a Fourier option pricing technique. C.W. Oosterlee M.J. Ruijter, M. Versteegh  
*The Journal of Computational Finance, Volume 19, Issue 1, 2015.*
- Unbiased simulation of stochastic differential equations. P.H. Labordere X. Tan, N. Touzi

We have benefited from the help of the engineer Cedric Doucet, supervised by Jérôme Lelong, for designing non regression tests for Premia.

## TOSCA Project-Team

## 6. New Software and Platforms

### 6.1. MOC

*Models Of Chemostat*

KEYWORD: Simulator

FUNCTIONAL DESCRIPTION: MOC (for Models of Chemostat) is a Python simulator of four chemostat models: a mass-structured stochastic individual based model, a mass-structured integro-differential model, the Crump-Young model and a system of ordinary differential equations. This software allows to simulate one or several of those models with different parameters, to plot graphics of evolution of biomass concentration, number of bacteria and substrate concentration as well as the phase portrait, to determine the law of the extinction time of the bacterial population in case of population extinction.

- Participants: Coralie Fritsch and Fabien Campillo
- Contact: Coralie Fritsch
- URL: <https://github.com/coraliefritsch/modelsOfChemostat>

### 6.2. AWFCController

*Acoustic Wind Farm Controller*

KEYWORDS: Matlab - Noise - Control

SCIENTIFIC DESCRIPTION: AWFCController is a matlab module dedicated to a real time application that performs acoustic control of wind farms based on microphones set near surrounding housings. It computes the optimal command for each wind turbine at each time-step to fulfil the law criteria of acoustic annoyance while maximizing the electric production. It uses local weather measurements (wind speeds and directions) and wind turbines noise estimates computed by an audio source separation algorithm on the acoustic measurements.

FUNCTIONAL DESCRIPTION: Nowadays, wind farm owners have to reduce the velocity of their wind turbines to comply with the regulation on acoustic annoyance. However, the variability of perceived noise due to weather variations makes optimization hard to achieve. AWFCController is developed along with an industrial project in order to improve the optimization by adapting wind turbines speeds in regards to acoustic measurements of permanent sensors. It computes optimal command from acoustic measurements and meteo data.

- Participants: Baldwin Dumortier, Emmanuel Vincent and Madalina Deaconu
- Contact: Baldwin Dumortier