RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2018

Section Software

Edition: 2019-03-07

ACUMES Project-Team

6. New Software and Platforms

6.1. 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: Concerning Chapter 1, 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. Concerning Chapters 2 and 3, the utilizer specifies cost and constraint functions by providing procedures compatible with Fortran 90. Chapter 3 does not require the specification of gradients, but only the functions themselves that are approximated by the software by quadratic meta-models.

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

6.2. 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

6.3. 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 Occulus Rift immersion.
NEWS OF THE YEAR: Demo movies are available from Youtube (see web site)

- Participants: Régis Duvigneau, Jean-Luc Szpyrka, David Rey, Clement Welsch and Abderrahmane Habbal
- Contact: Abderrahmane Habbal
- URL: 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: In 2018, the following points were addressed in AeroSol

* A 6 month CNRS contract, led by Vincent Perrier was obtained in the team Cagire, concentrated on the quality of the code. A two-year Inria Hub, led by Héloïse Beaugendre was obtained in the team Cardamom. On both of these contracts, Benjamin Lux was hired (January-June in Cagire team, and since October in Cardamom team). The library has kept on benefiting from the work of Florent Pruvost (Inria Hub HPCLib), on the continuous integration and packaging aspects.

* The CNRS contract, aiming at improving the code resulted in the successful porting from the inria gforge to the inria gitlab, with a functional pipeline of code assessment (based on Jenkins) and code quality assessment (based on sonarqube).

* Installation was simplified. A fully automatic installation script based on spack was developed.

* Development of a true documentation policy, based on a wiki. About half of the functional tests were documented and updated. Doxygen documentation was improved.

* An API was developed for the AeroSol library. The mesh reading, and parallel distribution was refactored.

* Update of the test case interface was updated by using this APIfor being more convenient. About half of the functional tests are now using this interface.

* Refactoring of the xml parameter file.

* Hyperbolized models, based on the hyperbolization of advection-diffusion models were added.

* Handling of nonconservative hyperbolic models.

* Improvement of mesh adaptation

* Beginning of implementation of droplet model for icing.

* Add the possibility of using several matrices, with a different number of variables

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

CARDAMOM Project-Team

6. New Software and Platforms

6.1. AeroSol

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

6.2. Crysa

KEYWORDS: Image analysis - 2D

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

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

6.3. Cut-ANOVA

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

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

6.4. Fmg

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

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

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

6.5. Mmg

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

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

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

Inside the volume, the software perform local mesh modifications (such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).
FUNCTIONAL DESCRIPTION: The Mmg plateform 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 convergency and edge lengths closest to 1) - the software behaviour in case of failure (warnings/error messages are printed only 1 time and there is no more exits in the code) - the mmg2d software that now uses the same structure than mmgs and mmg3d

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

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

6.6. MMG3D

Mmg3d
KEYWORDS: Mesh - Anisotropic - Mesh adaptation

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

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

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

Inside the volume, the software perform local mesh modifications (such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).
FUNCTIONAL DESCRIPTION: Mmg3d is one of the software of the Mmg platform. Is is dedicated to the modification of 3D volume meshes. It perform the adaptation and the optimization of a tetrahedral mesh and allow to discretize an isovalue.

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

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

6.7. NOMESH

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

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

6.8. ORComp

FUNCTIONAL DESCRIPTION: The ORComp platform is a simulation tool permitting to design an ORC cycle. Starting from the solar radiation, this plateform computes the cycle providing the best performance with optimal choices of the fluid and the operating conditions. It includes RobUQ , a simulation block of the ORC cycles, the 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

6. New Software and Platforms

6.1. 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: Houssem Haddar
- Contact: Houssem Haddar
- URL: http://sourceforge.net/projects/samplings-2d/

6.2. SAXS-LMA-HSPY

SAXS inversion using LMA and HSPY models
KEYWORD: SAXS measurements
FUNCTIONAL DESCRIPTION: This software determines nanoparticles size distribution from SAXS measurements (Small Angle X-ray Scattering). It contains two different approaches. The first one is based on a linear LMA model with automatic search for model parameters. The second approach uses a non-linear inversion of the HSPY model.

- Authors: Marc Bakry and Houssem Haddar
- Contact: Marc Bakry

6.3. FVforBlochTorrey

KEYWORDS: Simulation - PDE - Diffusion imaging - MRI
FUNCTIONAL DESCRIPTION: We developed a Matlab toolbox for solving the multiple-compartments Bloch-Torrey partial differential equation in 3D to simulate the water proton magnetization of a sample under the influence of diffusion-encoing magnetic field gradient pulses. We coupled the finite element spatial discretization with several ODE solvers in time that are available inside Matlab.

Result: the code will be made available on GitHub in 2019.

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

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 - Continued front-end for C++ based on Clang - Experimental support for building Abs-Normal Form tangent of non-smooth codes

- Participants: Laurent Hascoët and Valérie Pascual
- Contact: Laurent Hascoët
- URL: http://www-sop.inria.fr/tropics/tapenade.html

ELAN Team

5. New Software and Platforms

5.1. Argus-distribution

KEYWORDS: Frictional contact - Cloth dynamics - Mesh adaptation
SCIENTIFIC DESCRIPTION: The Argus-distribution software exactly replicates all the results published in the SIGGRAPH 2018 paper entitled "An Implicit Frictional Contact Solver for Adaptive Cloth Simulation", by Li et al. This paper presents the first method able to account for cloth contact with exact Coulomb friction, treating both cloth self-contacts and contacts occurring between the cloth and an underlying character. The key contribution is to observe that for a nodal system like cloth, the frictional contact problem may be formulated based on velocities as primary variables, without having to compute the costly Delassus operator. Then, by reversing the roles classically played by the velocities and the contact impulses, conical complementarity solvers of the literature can be adapted to solve for compatible velocities at nodes. To handle the full complexity of cloth dynamics scenarios, this base algorithm has been extended in two ways: first, towards the accurate treatment of frictional contact at any location of the cloth, through an adaptive node refinement strategy, second, towards the handling of multiple constraints at each node, through the duplication of constrained nodes and the adding of pin constraints between duplicata. This method allows to handle the complex cloth-cloth and cloth-body interactions in full-size garments with an unprecedented level of realism compared to former methods, while maintaining reasonable computational timings.allows to simulate cloth dynamics subject to frictional contact.
FUNCTIONAL DESCRIPTION: Adaptive cloth simulation in the presence of frictional contact. Reference software for the paper "An Implicit Frictional Contact Solver for Adaptive Cloth Simulation", Li et al. 2018, ACM Transactions on Graphics (SIGGRAPH'18).

- Participants: Jie Li, Gilles Daviet, Rahul Narain, Florence Descoubes, Matthew Overby, George Brown and Laurence Boissieux
- Partners: Department of Computer Science and Engineering, University of Minnesota - IIT Delhi
- Contact: Florence Descoubes
- Publication: An Implicit Frictional Contact Solver for Adaptive Cloth Simulation
- URL: http://www-users.cselabs.umn.edu/~lixx4611/contact_friction.html

GAMMA3 Project-Team

4. New Software and Platforms

4.1. ABL4FLO

Adaptive Boundary Layer 4 FLOw
KEYWORDS: Boundary layers - Hybrid meshes
FUNCTIONAL DESCRIPTION: ABL4FLO is a module used to perform adaptive boundary layer mesh adaptation as required in RANS solutions. It is included in Feflo.a/AMG-Lib software. It is based on a constrained version of the cavity operators in order to generate automatically hybrid elements. If a metric surface is provided, the normal and tangential direction are simultaneously adapted.

- Participant: Adrien Loseille
- Contact: Adrien Loseille
- Publications: Recent Improvements on Cavity-Based Operators for RANS Mesh Adaptation - Unstructured Mesh Generation and Adaptation - Robust Boundary Layer Mesh Generation
- URL: https://pyamg.saclay.inria.fr/

4.2. AMA4FLO

Anisotropic Mesh Adaptation 4 FLOw
KEYWORDS: 3D - Mesh adaptation
FUNCTIONAL DESCRIPTION: AMA4Flo is part of Feflo.a which is a robust anisotropic local remeshing software. It is intended for scientific computing with primary applications in aerodynamics and spatial studies. Surface and volume mesh adaptation are handled in a coupled-way. It also includes : - Boundary layers mesh generation for RANS simulations, - CAD re-projection and discrete surface remeshing, with - Hybrid mesh generation for boundary-layers - High-quality quasi-structured grids for complex geometries and complex corners: multi-normals, normals deactivation, ... - Highly anisotropic mesh adaptation, ratios up to 1 million are handled - Anisotropic/Boundary-layer coupling for supersonic shock/boundary layer interaction

The boundary layer module alone (abl4flo) is registered with the APP under nbr. IDDN. FR.001. 080032. 00.S.P.2012. 000.10000

initially, AMA4FLO was mainly focused on Computational Fluid Dynamics (4 FLOw), but it is now sed in many applications areas: seismic, reservoir engineering, spatial, hydrodynamics, hemodynamics, ...

- Participant: Adrien Loseille
- Contact: Adrien Loseille
- Publications: Very High Order Anisotropic Metric-Based Mesh Adaptation in 3D - Computational and Experimental Assessment of Models for the First AIAA Sonic Boom Prediction Workshop Using Adaptive High Fidelity CFD methods - Unique cavity-based operator and hierarchical domain partitioning for fast parallel generation of anisotropic meshes - Unstructured Mesh Generation and Adaptation - A Decade of Progress on Anisotropic Mesh Adaptation for Computational Fluid Dynamics - Metric-orthogonal Anisotropic Mesh Generation - Sonic Boom Assessment of a Hypersonic Transport Vehicle with Advanced Numerical Methods
- URL: https://pyamg.saclay.inria.fr/

4.3. BL2D

KEYWORDS: Abstraction - Meshing - Isotropic - Anisotropic - Delaunay - Mesher - Mesh

FUNCTIONAL DESCRIPTION: This software package stems from a former one called BL2D-V1. The meshing method is of controled 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 1ou 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/logiciels.html

4.4. BL2D-ABAQ

KEYWORDS: Anisotropic - Delaunay - Automatic mesher - Meshing - Mesher - Mesh
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 staisfying 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
- URL: http://pages.saclay.inria.fr/patrick.laug/logiciels/logiciels.html

4.5. BLGEOL

KEYWORDS: Automatic mesher - Geologic structure - Meshing - Mesher - Mesh
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: http://pages.saclay.inria.fr/patrick.laug/logiciels/logiciels.html

4.6. BLMOL

KEYWORDS: Mesher - Molecular surface - Meshing - Mesh
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/logiciels.html

4.7. BLSURF

KEYWORDS: Automatic mesher - Meshing - Mesher - Mesh
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: http://pages.saclay.inria.fr/patrick.laug/logiciels/logiciels.html

4.8. 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: https://www.rocq.inria.fr/gamma/Adrien.Loseille/index.php?page=softwares

4.9. 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

4.10. 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

4.11. 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

4.12. 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/

4.13. 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

4.14. VIZIR

Interactive visualization of hybrid, curbed and high-order mesh and solution
KEYWORD: Mesh
FUNCTIONAL DESCRIPTION: Vizir is a light, simple and interactive mesh visualization software, including : (i) A curved meshes visualizator: it handles high order elements and solutions, (ii) Hybrid elements mesh visualization (pyramids, prisms, hexahedra), (iii) Solutions visualization : clip planes, capping, iso-lines, iso-surfaces.

- Participants: Adrien Loseille and Rémi Feuillet
- Contact: Adrien Loseille
- Publication: Vizir: High-order mesh and solution visualization using OpenGL 4.0 graphic pipeline
- URL: http://vizir.inria.fr

4.15. 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: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html#Wolf-Nsc

4.16. 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: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

4.17. Wolf-Elast

KEYWORD: Scientific calculation
FUNCTIONAL DESCRIPTION: Wolf-Elast is a linear elasticity solver using the P1 to P3 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: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

4.18. 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: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

4.19. 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. High-order meshes are also handled

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Paul Louis George
- URL: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

4.20. 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: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

4.21. Wolf-Spyder

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

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: http://pages.saclay.inria.fr/frederic.alauzet/code_eng.html

MATHERIALS Project-Team

5. New Software and Platforms

5.1. 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-POST Team (section vide)

MINGUS Project-Team

6. New Software and Platforms

6.1. Selalib

SEmi-LAgrangian LIBrary
KEYWORDS: Plasma physics - Semilagrangian method - Parallel computing - Plasma turbulence
SCIENTIFIC DESCRIPTION: The objective of the Selalib project (SEmi-LAgrangian LIBrary) is to develop a well-designed, organized and documented library implementing several numerical methods for kinetic models of plasma physics. Its ultimate goal is to produce gyrokinetic simulations.

Another objective of the library is to provide to physicists easy-to-use gyrokinetic solvers, based on the semi-lagrangian techniques developed by Eric Sonnendrücker and his collaborators in the past CALVI project. The new models and schemes from TONUS are also intended to be incorporated into Selalib.
FUNCTIONAL DESCRIPTION: Selalib is a collection of modules conceived to aid in the development of plasma physics simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities from general and mathematical utilities and modules to aid in parallelization, up to pre-packaged simulations.

- Partners: Max Planck Insitute - Garching - Université de Strasbourg
- Contact: Philippe Helluy
- URL: http://selalib.gforge.inria.fr/

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/

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: The DIOGENeS software suite provides several tools and solvers for the numerical resolution of light-matter interactions at nanometer scales. A choice can be made between time-domain (DGTD solver) and frequency-domain (HDGFD solver) depending on the problem. The available sources, material laws and observables are very well suited to nano-optics and nano-plasmonics (interaction with metals). A parallel implementation allows to consider large problems on dedicated cluster-like architectures.

- Authors: Stéphane Lanteri, Nikolai Schmitt, Alexis Gobe and Jonathan Viquerat
- Contact: Stéphane Lanteri
- URL: https://diogenes.inria.fr/

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

5. New Software and Platforms

5.1. SAMSON

Software for Adaptive Modeling and Simulation Of Nanosystems
KEYWORDS: Bioinformatics - Simulation - Nanosystems - Structural Biology - 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/

5.2. 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/

5.3. 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/

5.4. Knodle

KNOwledge-Driven Ligand Extractor
KEYWORDS: Bioinformatics - Machine learning
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.

- Participants: Maria Kadukova and Sergey Grudinin
- Partner: MIPT Moscow
- Contact: Sergey Grudinin
- Publication: Knodle: A Support Vector Machines-Based Automatic Perception of Organic Molecules from 3D Coordinates
- URL: https://team.inria.fr/nano-d/software/Knodle/

5.5. 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
KEYWORD: Bioinformatics
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.

- Participants: Petr Popov and Sergey Grudinin
- Contact: Sergey Grudinin
- Publication: Rapid determination of RMSDs corresponding to macromolecular rigid body motions
- URL: https://team.inria.fr/nano-d/software/rigidrmsd/

5.6. SAMSON-Drug-design

KEYWORDS: Algorithm - Nanosystems - Structural Biology - Bioinformatics - Chemistry - 3D modeling - Molecular simulation
FUNCTIONAL DESCRIPTION: Arap Interpolation Path : Generate interpolation path between two protein structures by the As-Rigid-As-Possible principle from computer graphics

Ligand unbinding search : Find ligand unbinding pathway with the ART-RRT method. The method uses the T-RRT method from robotics for efficiently searching low-energy paths and the ARAP modeling method from computer graphics for handling flexible motions of the ligand and reducing the number of thedimensions of the search space.

Protein Path search : Find protein conformational transition paths between two given conformations with the ART-RRT method. The method uses the T-RRT method from robotics for searching low-energy paths and the As-Rigid-As-Possible (ARAP) methods from computer graphics for handling the flexibility of the protein and reducing the number of the dimensions of the search space.

- Authors: Leonard Jaillet, Minh Khoa Nguyen and Jocelyn Gaté
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.7. DeepSymmetry

KEYWORDS: Bioinformatics - 3D modeling - Machine learning - Neural networks
FUNCTIONAL DESCRIPTION: DeepSymmetry is a method based on three-dimensional (3D) convolutional networks that detects structural repetitions in proteins and their density maps. It identifies tandem repeat proteins, proteins with internal symmetries, their symmetry order, and also the corresponding symmetry axes.

- Participants: Guillaume Pages and Sergey Grudinin
- Contact: Sergey Grudinin
- Publication: DeepSymmetry : Using 3D convolutional networks for identification of tandem repeats and internal symmetries in protein structures
- URL: https://team.inria.fr/nano-d/software/deepsymmetry/

5.8. SAMSON-ARAP-Planner

KEYWORDS: 3D - Algorithm - Nanosystems - Bioinformatics - Structural Biology - Chemistry
FUNCTIONAL DESCRIPTION: ARAP planner combines the ARAP method from computer graphics with T-RRT exploration method from robotics for efficiently finding low-energy paths in high-dimensional energy landscapes.

- Authors: Leonard Jaillet and Minh Khoa Nguyen
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.9. SAMSON-Hydrocarbons

KEYWORDS: Algorithm - Quantum chemistry - Chemistry - Nanosystems - 3D - 3D modeling
FUNCTIONAL DESCRIPTION: Interactive quantum chemistry : This SAMSON Element demonstrates interactive quantum chemistry for small molecules at the ASED-MO level of theory. Choose the ASED-MO (atom superposition and electron delocalization) interaction model when adding a simulator through the 'Simulation' menu. The SAMSON Element also includes an App that makes it possible to visualize how the electron density evolves during interactive simulation.

Brenner interction model : This SAMSON Element contains an adaptive implementation of the Brenner interaction model. Interaction models are one of the five model categories that are used to model nanosystems in SAMSON, along with structural models (for geometry and topology), dynamical models (to represent degrees of freedom), visual models (for visual representations) and property models (to represent properties). The Brenner interaction model is a reactive bond-order potential for hydrocarbon systems. This adaptive implementation makes it possible to interactively simulate large systems. Choose this interaction model when adding a simulator through the 'Simulation' menu.

- Author: Maël Bosson
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.10. SAMSON-RDKit

KEYWORDS: 2D - 3D - Chemistry - Algorithm - 3D modeling - Structural Biology - Bioinformatics

FUNCTIONAL DESCRIPTION: Based on the RDKit open-source libraries, convert and manage SMILES codes in the SAMSON platform. The RDKit-SMILES Manager element allows you to easily import files (.smi or .txt) containing several SMILES codes or add each code separately. 2D conformation of each code will then be generated and you can save them into svg or png files. Using a checkbox you will be able to select the codes that you want to convert into 3D structures and add them directly into the SAMSON data graph node as structural model. For more information about using this SAMSON Element, please visit https://documentation.samson-connect.net/using-the-rdkit-smiles-manager/.

- Author: Yassine Naimi
- Partner: Inria
- Contact: Stéphane Redon
- URL: https://samson-connect.net/app/main?key=element&uuid=ce09650a-c071-4e84-1f6a-b8706937d5c1

5.11. SAMSON-GROMACS

KEYWORDS: Algorithm - Materials - Chemistry - Bioinformatics - Structural Biology - Nanosystems - 3D modeling - 3-order
FUNCTIONAL DESCRIPTION: This SAMSON Element wraps GROMACS 5.1 force fields and setup tools. Use the "GROMACS setup" app (in the App menu), which wraps the pdb2gmx tool, to generate a structural model suitable for simulation (i.e. add hydrogens, etc.). Then, apply a simulator from the Simulation menu and choose "GROMACS force field" to add a GROMACS interaction model suitable for interactive minimization and simulation (no periodic boundary conditions). Note that, at the moment, at most one structural model should be selected (or in the document, when the selection is empty), and that bond lengths are not yet constrained in this version. This may be combined with the Twister editor to perform large-scale modifications of the structure, and the secondary structure visual model for interactively updated secondary structure prediction. Future updates of this SAMSON Element will wrap more GROMACS tools. Source code for this SAMSON Element will be made available at https://gforge.inria.fr/projects/elements/.

- Authors: Stéphane Redon, Minh Khoa Nguyen and Yassine Naimi
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.12. SAMSON-Essentials

KEYWORDS: 3D - C++ - OpenGL - Molecular surface - Molecular simulation - Structural Biology - Chemistry - 3D modeling - Bioinformatics - Nanosystems
FUNCTIONAL DESCRIPTION: A set of SAMSON Elements that adds essential features to SAMSON such as import / export of models, import / export of documents, generators, simulators, editors, scripting, app as well as software integrations (autodock vina).

- Authors: Stéphane Redon, Jocelyn Gaté, Guillaume Pages, Dmitriy Marin, Svetlana Artemova, Himani Singhal, Marc Aubert, Marc Piuzzi and Clement Beitone
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.13. Samson-base

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

- Participants: Evelyne Altariba, Jocelyn Gaté, Noëlle Le Delliou and Stéphane Redon
- Contact: Stéphane Redon

5.14. SAMSON-Connect

KEYWORDS: Web Application - Software platform - Web
FUNCTIONAL DESCRIPTION: SAMSON, SAMSON Elements and the SAMSON Software Development Kit are distributed via the SAMSON Connect website.[2] The site acts as a repository for the SAMSON Elements being uploaded by developers, and users of SAMSON choose and add Elements from SAMSON Connect.

- Authors: Stéphane Redon, Mohamed Yengui and Jocelyn Gaté
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.15. SAMSON-Updater

KEYWORDS: Webservices - Web Application
FUNCTIONAL DESCRIPTION: Web service to ensure communication between SAMSON and SAMSON-Connect. Features: Add / remove new items to SAMSON if they have been added / deleted on SAMON-Connect Update SAMSON or SAMSON-Elements Authenticate users ...

- Authors: Mohamed Yengui and Jocelyn Gaté
- Partner: Inria
- Contact: Stéphane Redon

5.16. SAMSON-Various-tools

SAMSON-Various-toolsrere
KEYWORDS: 3D - 3D modeling - Chemistry - Algorithm - Bioinformatics - Nanosystems - Structural Biology
FUNCTIONAL DESCRIPTION: Cluster Game : This element has been made in order to help students discover the Lennard Jones interactions. It is a game in which the goal is to optimize the atoms' placement. Contains eight levels and five tutorial levels.

Atoms Selector : This SAMSON element allows selection of atoms in the active document according to a user-provided expression with the usage of NSL-like variables (NSL - Node Specification Language), standard mathematical and logical operations. Parsing and evaluation of expressions is done with the usage of C++ Mathematical Expression Parsing And Evaluation Library 'exprtk' by Arash Partow (https://github.com/ArashPartow/exprtk)

Simple Script : This SAMSON element allows modification of some parameters of atoms using scripting language, standard mathematical and logical operations, and NSL-like variables (NSL - Node Specification Language). The script is applied to each atom independently. Parsing and evaluation of the script is done with the usage of C++ Mathematical Expression Parsing And Evaluation Library 'exprtk' by Arash Partow (https://github.com/ArashPartow/exprtk)

Bond Angle Distribution : This App will compute the bond angle distribution of the selected atoms. The result and its image can then be exported.

Bond Distortion Visualisation : This App permits to visualize with colors the distortion of a molecular or crystalic structure. The angle distortion, the bond distortion and the projected bond distortion can be represented with colors on bonds and atoms.

Frame axis : Basic visual model to show cartesian axis. Open a new visual model and select "Frame axis" to see the frame axis as arrows, lines or both.

Radial Distribution Function : This app computes and draws the radial distribution function of a selection. - Compute the crossed-RDF by selecting 2 different sets of atoms. - Follow the evolution of the RDF by selecting a simulator.

Adaptive Lennard-Jones : An interaction model to compute the forces with an adaptive version of Lennard-Jones potential. The update of forces is done by storing all the position, and at each position update, subtracting previous pair forces, then adding new ones. If both pair particles were frozen by restraining dynamical model, the update is useless and so not done.

STL File Importer : Reads Stereolithography (.stl) binary and ASCII files. Spawns carbon atoms at the intersections of vertices to create quickly new original atomic configurations. Many STL files are avalaible online to generate thousands of new configurations.

StyleSheet Viewer : An app for internal developers to test their skin/styles ...

Animation Player : Create animation from a list of conformations in SAMSON Document view There are 3 play modes: loop, only 1 time, or continuous back-forth. The user can change the frame order by drag and drop in the frame list.

Internal Coordinate Editor : This editor rotate the molecule by defining rotation axis and rotation angle. The user define the rotation axis (represented by an arrow in the view) by clicking on one atom and drag it to the second atom. The rotation angle is defined by the small GUI windows. The editor will try to rotate all the atoms after the head of the arrow and in between the tail and head of the arrow

RMSD : This app calculates RMSD between 2 structures. If it is an amino acid chains, a sequence alignment of the structures is needed (in fasta format). The fasta format has to be obtained from external sources. If it is not a protein, the app will try to match atoms one by one in both structures.

Trajectory Importer : This app import selected pdb files (hold Ctrl + Mouse click for multiple selection) as a trajectory. The result is one single structural model and a list of conformations in SAMSON Document View

Open Babel connector : This app allows users to use Open Babel from inside SAMSON

ARPS demo : This SAMSON Element features a demonstration of ARPS: Adaptively Restrained Particle Simulations, an adaptive simulation technique able to focus computations on the most mobile degrees of freedom. In this demo, a collision cascade may be simulated with various degrees of precision by changing the restrained dynamics threshold and the full dynamics threshold. For example, 0 0 produces a classical, non-adaptive simulation, while 0.625 and 0.7 result in a 10 times speedup in this example (without the graphics overhead). Click on 2D Shock to generate the example, enter the simplification parameters, and press start to simulate the collision cascade. Undo and redo make it possible to zoom on and compare simulations. Please refer to "S. Artemova and S. Redon. Adaptively restrained particle simulations. Physical review letters, 2012" for more details.

Hydrogen bond finder : Find hydrogen bonds in a given structure. The bonds is detected by specifying a threshold distance. Bonds are displayed by yellow lines.

Lennard-Jones model : This SAMSON Element contains a Lennard-Jones interaction model that may be used for several purposes: teaching, learning about van der Waals interactions, developing optimization algorithms, looking for minimum energy Lennard-Jones clusters through interactive simulation, etc. Add this force field to a group of atoms (the atom types do not matter) via the 'Simulation' menu.

Catalogue : BETA version. Bunch of structures easy to load, with images.

Catalogue Generator : BETA. Generator for the Catalogue module.

SAMSON Basic Tutorial : Tutorial for SAMSON : Basic functionnalities. Learn how to create, move and delete an atom, and then create a basic molecule thanks to a step-by-step guide. Experiment in sandbox mode. Test your mastery of SAMSON's tools with 4 speed challenges. The following elements are required : SAMSON Editors, Periodic table, Basic importers. Currently only available in french.

SAMSON Courses : BETA. Module with a custom display, depending on the entry files

SAMSON Courses Creator : BETA. Generator for SAMSON Course module

Charts : A SAMSON Element to allow user plotting something from SAMSON datas interactively

Leap : A driver to control SAMSON with the Leap motion controller

- Authors: Mohamed Nadhir Ben Hadj Abdellatif, Svetlana Artemova, Clement Beitone, Jocelyn Gaté, Dmitriy Marin, Pierre Mehaye, Minh Khoa Nguyen, Guillaume Pages, Stéphane Redon, François Rousse and Joachim Woerly-Moussier
- Partner: Inria
- Contact: Stéphane Redon

5.17. SAMSON-Crystal-Study-Pack

KEYWORDS: Algorithm - Nanosystems - 3D - 3D modeling - Physical simulation
FUNCTIONAL DESCRIPTION: CrystalConstrainer : Constrains borders of a crystal. The crystal should be alignes on xyz axes. The margen defines the maximum distance to the bonding box border for which atoms are constrained. Can use the current positions as constrained pos or some fixed one. Can Constrain each pair of plans separately or by couples (e.g. XY)

CrystalProber : Get some statistics about a crystal. Compute for now the X, Y and Z lattice parameters. Can remove a margen to discard atoms at the border

CrystalRigidityProber : Analyze some crystal properties related to the rigidity and based on forces, such as the Young modulus, Poisson's ration, elastic constants, stiffness, etc.

Keating : Implement the Keating force field. Compute energy and forces according to positions. Follows anikin2011keating

nonharmonic Keating : Develop a nonharmonic Keating model as proposed in Rucker1995anharmonic. As parameter file it uses a .nhk extension. As parameters, it require a nu and theta0 value in addition to the equilibrium distances for each atom type. Also, it requires a0 distances for pairwise atoms, in addition to the alpha and beta parameters.

generalized harmonic Keating : Develop a generalized harmonic Keating force field as proposed in mojica2010modelisation. This model generalizes to atoms of columns III and V of the periodic table. The systems are anisotropics, with specific bond lengths and angles when involving the z direction.

CrystalCharacterizer : Provides functionalities to characterise a crystal.

CrystalVisualizer : Provides functionalities to visualize a crystal. Choose the pointing direction of the eye, according to some representative directions of the crystal mesh. Choose the orientation in the camera planer.

- Author: Leonard Jaillet
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.18. SAMSON-Materials

KEYWORDS: Algorithm - Materials - 3D - 3D modeling - Nanosystems
FUNCTIONAL DESCRIPTION: Crystal Creator : This SAMSON Elements enables to generate crystals. It contains a SAMSON App to write a unit cell and a SAMSON importer to read CIF format files. Once a unit cell is written or imported, it can be repeated in the directions of the lattice vectors to create a whole crystal. Each repetition is not a mere copy but is generated again so that the defects and the impurities are modeled. A functionality of the associated property model permits to cut the crystal with the Miller indices and expose the important crystalic planes.

Orbital Free DFT : This App computes the electron density of an atomic system. It comes with an interaction model to minimize the atomic structure and a visual model to appreciate the result of computations. The scheme used is the orbital-free DFT, and the pseudo-potential available restrains its use to only 9 elements : Li, Mg, Al, Si, P, Ga, In and Sb.

- Author: François Rousse
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.19. SAMSON-Planner-Tools

KEYWORDS: 3D - Algorithm - 3D modeling - Molecular simulation - Chemistry - Planning
FUNCTIONAL DESCRIPTION: A set of SAMSON Elements that adds planning features to SAMSON.

- Author: Leonard Jaillet
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

5.20. SAMSON-HEX

KEYWORD: Algorithm
FUNCTIONAL DESCRIPTION: Sampling and Docking using the Hex algorithm developed by Dave Ritchie in SAMSON. Docking solutions can be easily displayed and clustered.

- Authors: Sergey Grudinin, Emilie Neveu and Yassine Naimi
- Partner: Inria
- Contact: Stéphane Redon
- URL: https://www.samson-connect.net/

5.21. SAMSON-UFF

KEYWORDS: Algorithm - Bioinformatics - 3D - 3D modeling - Nanosystems - Molecular simulation
FUNCTIONAL DESCRIPTION: Universal Force Field : This SAMSON Element contains a new implementation of the Universal Force Field, with automatic structure perception. In order to use this interaction model, add a simulator to the document from the Simulation menu, and choose "Universal Force Field". The property window of the interaction model makes it possible to customize the perception and setup the interaction model (e.g. choose the cutoff), and displays the various energy types and the total energy.

Interactive Modeling Universal Force Field : It is an extension of UFF that combines the possibility to significantly modify molecular structures (as with reactive force fields) with a broad diversity of supported systems thanks to the universality of UFF. Such an extension lets the user easily build and edit molecular systems interactively while being guided by physics based inter-atomic forces.

- Authors: Leonard Jaillet and Svetlana Artemova
- Partner: Inria
- Contact: Stéphane Redon
- URL: https://samson-connect.net/app/main?key=element&uuid=8cbdc8b1-59e1-6459-d68f-b840275dd5e9

5.22. SAMSON-Normal-modes

KEYWORDS: Algorithm - Bioinformatics - Structural Biology - 3-order - 3D modeling - Nanosystems

FUNCTIONAL DESCRIPTION: Normal mode analysis advanced : This SAMSON Element computes the nonlinear normal modes of a molecular system (protein, RNA, DNA) very quickly using the NOLB algorithm developed by Alexandre Hoffmann and Sergei Grudinin (J. Chem. Theory Comput., 2017, 13 (5), pp 2123-2134, DOI: 10.1021 / acs.jctc.7b00197.). The user indicates the desired number of modes, the interactions cutoff distance and the potential function. For now, the elastic network model potential is the one that is available. In the output, each mode is represented by a slider. The user can visualize the motion of each mode independently by moving its corresponding slider manually or by checking its checkbox and then pressing on the play button. Also, the user can visualize the motion of a combination of modes selecting them before playing the motion. The transformations used in this motion can be set to linear or nonlinear and the amplitude of the motion can be increased/decreased by changing the scaling factor. During this motion, the user can activate a real time minimization using one of the provided algorithms (steepest descent, conjugated gradient or LBGF) and defined values of minimization steps and minimization tolerance. Finally, the user can either save/export a given conformation of the structure or the entire displayed trajectory by going into the "Save Frames" tabulation of the SAMSON element. Please visit https://blog.samson-connect.net/computing-non-linear-normal-modes-of-biomolecules/ for a tutorial.

Normal mode analysis : A light version of the previous element

- Authors: Sergey Grudinin, Alexandre Hoffmann and Yassine Naimi
- Partner: Inria
- Contact: Sergey Grudinin
- URL: http://samson-connect.net

5.23. SAMSON-SAXS

KEYWORDS: Algorithm - Bioinformatics - Structural Biology - Nanosystems - 3D - 3D modeling
FUNCTIONAL DESCRIPTION: The Pepsi-SAXS module rapidly computes small-angle X-ray scattering profiles. It is based on the spherical harmonics expansion method and interactively updates the fits if the molecular structure is modified. Multi-threading is currently only supported for Linux & macOS.

- Authors: Sergey Grudinin, Mariya Garkavenko and Mohamed Nadhir Ben Hadj Abdellatif
- Partner: Inria
- Contact: Sergey Grudinin
- URL: https://samson-connect.net/app/main?key=element&uuid=844be03b-cab2-4420-464b-6f0f9384bc4a

5.24. Ananas

Analytical Analyzer of Symmetries
KEYWORDS: Bioinformatics - Structural Biology
FUNCTIONAL DESCRIPTION: Analytical Analyzer of Symmetries is a software for detection and assessment of the quality of symmetry in a protein assembly.

This software can : Detect the best axes of symmetry for any symmetry group in an assembly containing the right amount of chains, Provide the symmetry-aware RMSD for these axes, Detect the best axis of symmetry for cyclic assemblies with missing subunits, Compute the axes of symmetry with user-provided correspondences.

- Participants: Guillaume Pages and Sergey Grudinin
- Contact: Sergey Grudinin
- Publications: Analytical symmetry detection in protein assemblies. I. Cyclic symmetries - Analytical symmetry detection in protein assemblies. II. Dihedral and Cubic symmetries
- URL: https://team.inria.fr/nano-d/software/ananas/

5.25. Pepsi-SAXS

KEYWORDS: Bioinformatics - Structural Biology - Data modeling
FUNCTIONAL DESCRIPTION: Pepsi-SAXS (PEPSI stands for Polynomial Expansions of Protein Structures and Interactions) is new implementation of the multipole-based scheme initially proposed by Stuhrmann (Stuhrmann, 1970). Overall, our method is significantly faster with a similar accuracy compared to Crysol, FoXS, and the 3D-Zernike implementation from the SAStbx package.

- Participant: Sergey Grudinin
- Partner: MIPT Moscow
- Contact: Sergey Grudinin
- Publication: Pepsi-SAXS : an adaptive method for rapid and accurate computation of small-angle X-ray scattering profiles
- URL: https://team.inria.fr/nano-d/software/pepsi-saxs/

5.26. NOLB

NOn-Linear rigid Block NMA method
KEYWORDS: Structural Biology - Bioinformatics - Elasticity - Proteins - Motion analysis
FUNCTIONAL DESCRIPTION: It's a new conceptually simple and computationally efficient method for non-linear normal mode analysis of macromolecules.

- Participants: Sergey Grudinin and Alexandre Hoffmann
- Contact: Sergey Grudinin
- Publications: NOLB: Nonlinear Rigid Block Normal Mode Analysis Method - RapidRMSD: Rapid determination of RMSDs corresponding to motions of flexible molecules
- URL: https://team.inria.fr/nano-d/software/nolb-normal-modes/

5.27. SBROD

KEYWORDS: Bioinformatics - Machine learning
FUNCTIONAL DESCRIPTION: Smooth orientation-dependent scoring function (SBROD) for coarse-grained protein quality assessment uses only the conformation of the protein backbone, and hence it can be applied to scoring the coarse-grained protein models.

The workflow of SBROD consists in two stages. First, the method extracts features from each protein model in the dataset. Then, the scoring function assigns a score to each processed protein model depending on its features extracted at the first stage. Figure above schematically shows the workflow of SBROD. Here, four types of inter-atomic interactions, described in details below, are taken into account when extracting the features. After these features have been extracted and preprocessed, a Ridge Regression model is trained on them to predict the GDT-TS of protein models.

- Participants: Mikhail Karasikov, Guillaume Pages and Sergey Grudinin
- Contact: Sergey Grudinin
- Publication: Smooth orientation-dependent scoring function for coarse-grained protein quality assessment
- URL: https://team.inria.fr/nano-d/software/sbrod/

5.28. Ornate

KEYWORDS: Bioinformatics - Machine learning - Neural networks

FUNCTIONAL DESCRIPTION: Oriented Routed Neural network with Automatic Typing is a method for protein quality assessment. Ornate is a residue-wise scoring method. It first constructs a three dimensional map representing the structure of the residue, and its neighborhood.

- Participants: Guillaume Pages, BENOIT CHARMETTANT and Sergey Grudinin
- Contact: Sergey Grudinin
- Publication: Protein model quality assessment using 3D oriented convolutional neural networks
- URL: https://team.inria.fr/nano-d/software/ornate/

5.29. SAMSON-AR-LAMMPS

KEYWORDS: Algorithm - Molecular simulation - 3D modeling

- Authors: Sémého Edorh, Krishna Kant Singh and Dmitriy Marin
- Partner: Inria
- Contact: Stéphane Redon
- URL: http://samson-connect.net

RAPSODI Project-Team

6. New Software and Platforms

6.1. Platform NS2DDV-M

NS2DDV-M is a Matlab code, developed by C. Calgaro Zotto, E. Creusé, and A. Mouton (CNRS research engineer at Université de Lille), for the simulation of homogeneous and inhomogeneous fluid flows by a combined Finite Volume-Finite Element method. The code is freely distributed, to allow for easy comparisons with concurrent codes on benchmark test-cases, and to promote new collaborations in the domain.
In 2018, a new version (v. 2.0) has been released, which contains a detailed documentation as well as some new functionalities, such as some post-processing tools and parallel computation capabilities.

CAGE Project-Team (section vide)

COMMANDS Project-Team

6. New Software and Platforms

6.1. BOCOP

Boite 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

5. New Software and Platforms

5.1. FEMMES

KEYWORD: Linear system
FUNCTIONAL DESCRIPTION: The Software FEMMES makes it possible to perform simulations for observers which converge to the exact value of the solutions of a studied system in finite time. The considered systems are linear continuous-time time-invariant systems.

- Partner: Inria
- Contact: Frédéric Mazenc

FACTAS Team

5. New Software and Platforms

5.1. pisa

KEYWORDS: Electrical circuit - Stability
FUNCTIONAL DESCRIPTION: To minimise prototyping costs, the design of analog circuits is performed using computer-aided design tools which simulate the circuit's response as accurately as possible.

Some commonly used simulation tools do not impose stability, which can result in costly errors when the prototype turns out to be unstable. A thorough stability analysis is therefore a very important step in circuit design. This is where pisa is used.

pisa is a Matlab toolbox that allows designers of analog electronic circuits to determine the stability of their circuits in the simulator. It analyses the impedance presented by a circuit to determine the circuit's stability. When an instability is detected, pisa can estimate location of the unstable poles to help designers fix their stability issue.

RELEASE FUNCTIONAL DESCRIPTION: First version

- Authors: Adam Cooman, David Martinez Martinez, Fabien Seyfert and Martine Olivi
- Contact: Fabien Seyfert
- Publications: Model-Free Closed-Loop Stability Analysis: A Linear Functional Approach - On Transfer Functions Realizable with Active Electronic Components
- URL: https://project.inria.fr/pisa

5.2. PUMA-HF

PUMA-HF: Passive Uniform Matching
KEYWORD: Transfer functions
FUNCTIONAL DESCRIPTION: PUMA computes a passive rational 2-port filtering function presenting a reference impedance (i.e. 50 Ohm) at the first port, and the conjugate of the given load impedance within a frequency band at the second port.

- Authors: David Martinez Martinez, Adam Cooman, Martine Olivi and Fabien Seyfert
- Partners: Xlim - DGA-MI - CNES
- Contact: Fabien Seyfert
- Publication: Synthesis Method for Matching Filters
- URL: https://project.inria.fr/puma/

I4S Project-Team (section vide)

MCTAO Project-Team

6. New Software and Platforms

6.1. Hampath

KEYWORDS: Optimal control - Second order conditions - Differential homotopy - Ordinary differential equations
FUNCTIONAL DESCRIPTION: Hampath is a software developped 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). It has a Fortran kernel, uses Tapenade (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: Experimentation - Motion analysis - Sensors - Performance analysis - 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/

NON-A POST Team

5. New Software and Platforms

5.1. ADHOMFI

Adaptive Homogeneous Filtering
KEYWORDS: Automatic differentiation - Filtering
FUNCTIONAL DESCRIPTION: allows to reconstruct a signal based on derivatives estimation and to filter high amplitude and wide frequencies spectrum perturbations.

- Contact: Denis Efimov

QUANTIC Project-Team (section vide)

SPHINX Project-Team

5. New Software and Platforms

5.1. 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

5.2. GPELab

Gross-Pitaevskii equations Matlab toolbox
KEYWORDS: 3D - Quantum chemistry - 2D
FUNCTIONAL DESCRIPTION: GPELab 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/

TRIPOP Team

5. New Software and Platforms

5.1. Platforms: SICONOS

5.1.1. Platform A : SICONOS

Participants: Vincent Acary, Maurice Brémond, Olivier Huber, Franck Pérignon.

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, intercations, 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/

TROPICAL Project-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
- Publications: A Formalization of Convex Polyhedra Based on the Simplex Method - A Formalization of Convex Polyhedra Based on the Simplex Method - First steps in the formalization of convex polyhedra in Coq
- URL: https://github.com/nhojem/Coq-Polyhedra

BONUS Team

6. New Software and Platforms

6.1. Platforms

6.1.1. Grid'5000 testbed: extension with GPUs at Lille

KEYWORDS: Experimental testbed, large-scale computing, high-performance computing, GPU computing, cloud computing, big data
FUNCTIONAL DESCRIPTION: Grid'5000 is a project initiated in 2003 by the French government to promote scientific research on large scale distributed systems. The project is later supported different research organizations including Inria, CNRS, the french universities, Renater which provides the wide-area network, etc. The overall objective of Grid'5000 was to build by 2007 a nation-wide experimental testbed composed of at least 5000 processing units and distributed over several sites in France. From a scientific point of view, the aim was to promote scientific research on large-scale distributed systems.
Grid'5000 was installed at the center of IT resources including supercomputing resources of Université de Lille 1 and opened to users in 2005. Since March 2017, the Grid'5000 site has moved to the premises on Inria Lille within the context of the phase 1 of the CPER data program (see Section 9.1) with a completely new hardware equipment. As a scientific leader of the testbed for the Lille's site, N. Melab has been strongly involved in the extension (phase 2 of CPER data) of the platform with 16 computing serveurs, 16 Nvidia GPUs (12 P100 and 4V100), 2 storage serveurs 200TB and 2 administration servers. Grid'5000 at Lille is used by more than 150 users including 100 external ones. The testbed is used for research as well as for teaching allowing a high scientific production (publications, PhD theses, etc.) and over 30 master students to get started with parallel and distributed programming.

- Participants: N. Melab, external collaborators: D. Delabroy, T. Peltier, L. Nussbaum.
- 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 impredictability 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: svn+ssh://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 speach 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 unpredictible 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

6.6. ProximalDenoising

KEYWORDS: 2D - Image filter - Filtering - Minimizing overall energy - Noise - Signal processing - Image reconstruction - Image processing
SCIENTIFIC DESCRIPTION: Image filtering is contemplated in the form of a sparse minimization problem in a non-convex setting. Given an input image I, one seeks to compute a denoised output image u such that u is close to I in the L2 norm. To do so, a minimization term is added which favors sparse gradients for output image u. Imposing sparse gradients lead to a non-convex minimization term: for instance a pseudo-norm Lp with $0 < p < 1$ or a Cauchy or Welsh function. Half-quadratic algorithm is used by adding a new variable in the minimization functionnal which leads to two sub-problems, the first sub-problem is non-convex and solved by use of proximal operators. The second sub-problem can be written in variational form, and is best solved in Fourier space: it takes the form of a deconvolution operator whose kernel can be approximated by a finite sum of separable filters. This solution method produces excellent computation times even on big images.
FUNCTIONAL DESCRIPTION: Use of proximal and non quadratic minimization. GPU implementation.

RELEASE FUNCTIONAL DESCRIPTION: This software implements H. Badri PhD thesis results.

- Authors: Marie Martin, Chiheb Sakka, Hussein Yahia, Nicolas Brodu, Gabriel Augusto Zebadua Garcia and Khalid Daoudi
- Partner: Innovative Imaging Solutions I2S
- Contact: Hussein Yahia
- URL: https://gitlab.inria.fr/marmarti/i2s_geostat_C

INOCS Project-Team

6. New Software and Platforms

6.1. 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

6.2. KEOLIS-MEDIATOUR

KEYWORDS: Operational research - Mathematical Optimization - Staff scheduling
FUNCTIONAL DESCRIPTION: This software is a prototype developed under a bilateral contract with the company Keolis. This software is a solver which aims to optimize the scheduling of mediation staff More precisely, for each member of the mediation staff working in a public transportation network, MEDIATOUR determines his/her schedule along the day, i.e. when and where he/she is present. Various operational constraints must be taken into account such as the coverage of the network. This software is designed to solve large-scale industrial instances (the subway network of Lille) in short computation times (less than 1 minute).

- Contact: Frédéric Semet

6.3. 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

MISTIS Project-Team

6. New Software and Platforms

6.1. BOLD model FIT

KEYWORDS: Functional imaging - FMRI - Health
SCIENTIFIC DESCRIPTION: Physiological and biophysical models have been proposed to link neuronal activity to the Blood Oxygen Level-Dependent (BOLD) signal in functional MRI (fMRI). Those models rely on a set of parameter values that are commonly estimated using gradient-based local search methods whose initial values are taken from the literature. In some applications, interesting insight into the brain physiology or physiopathology can be gained from an estimation of the model parameters from measured BOLD signals. In this work we focus on the extended Balloon model and propose the estimation of 15 parameters using seven different approaches: three versions of the Expectation Maximization Gauss-Newton (EM/GN) approach (the *de facto* standard in the neuroscientific community) and four metaheuristics (Particle Swarm Optimization (PSO), Differential Evolution (DE), Real-Coded Genetic Algorithms (GA), and a Memetic Algorithm (MA) combining EM/GN and DE). To combine both the ability to escape local optima and to incorporate prior knowledge, we derive the target function from Bayesian modeling. The general behavior of these algorithms is analyzed and compared, providing very promising results on challenging real and synthetic fMRI data sets involving rats with epileptic activity. These stochastic optimizers provided a better performance than EM/GN in terms of distance to the ground truth in 4 out of 6 synthetic data sets and a better signal fitting in 12 out of 12 real data sets. Non-parametric statistical tests showed the existence of statistically significant differences between the real data results obtained by DE and EM/GN. Finally, the estimates obtained from DE for these parameters seem both more realistic and more stable or at least as stable across sessions as the estimates from EM/GN. This is the largest comparison of optimizers for the estimation of biophysical parameters in BOLD fMRI
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
NEWS OF THE YEAR: The main differences with our previous work: 1) we also use synthetic data, 2) we use stochastic GN and MCMC+DE, 3) We evaluate results not only in physiological terms but also comparing fitness function values. Also changes were made to allow running on the cluster via MPI

- Participants: Pablo Mesejo Santiago, Florence Forbes and Jan Warnking
- Partner: University of Granada, Spain
- Contact: Pablo Mesejo Santiago
- Publication: A differential evolution-based approach for fitting a nonlinear biophysical model to fMRI BOLD data
- URL: https://hal.archives-ouvertes.fr/hal-01221115v2/

6.2. PyHRF

KEYWORDS: Medical imaging - Health - Brain - IRM - Neurosciences - Statistic analysis - FMRI
SCIENTIFIC DESCRIPTION: Functional Magnetic Resonance Imaging (fMRI) is a neuroimaging technique that allows the non-invasive study of brain function. It is based on the hemodynamic variations induced by changes in cerebral synaptic activity following sensory or cognitive stimulation. The measured signal depends on the variation of blood oxygenation level (BOLD signal) which is related to brain activity: a decrease in deoxyhemoglobin concentration induces an increase in BOLD signal. The BOLD signal is delayed with respect to changes in synaptic activity, which can be modeled as a convolution with the Hemodynamic Response Function (HRF) whose exact form is unknown and fluctuates with various parameters such as age, brain region or physiological conditions. In this work we propose to analyze fMRI data using a Joint Detection-Estimation (JDE) approach. It jointly detects cortical activation and estimates the HRF. In contrast to existing tools, PyHRF estimates the HRF instead of considering it as a given constant in the entire brain.

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.
NEWS OF THE YEAR: The framework to perform software tests has been further developed. Some unitary tests have been set.

- 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
- Publications: Frontiers in Neuroinformatics Flexible multivariate hemodynamics fMRI data analyses and simulations with PyHRF - Fast joint detection-estimation of evoked brain activity in event-related fMRI using a variational approach - A Bayesian Non-Parametric Hidden Markov Random Model for Hemodynamic Brain Parcellation
- URL: http://pyhrf.org

6.3. xLLiM

High dimensional locally linear mapping
KEYWORDS: Clustering - Regression
SCIENTIFIC DESCRIPTION: Building a regression model for the purpose of prediction is widely used in all disciplines. A large number of applications consists of learning the association between responses and predictors and focusing on predicting responses for the newly observed samples. In this work, we go beyond simple linear models and focus on predicting low-dimensional responses using high-dimensional covariates when the associations between responses and covariates are non-linear.
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.
NEWS OF THE YEAR: A new Hierarchical version of GLLiM has been developed in collaboration with University of Michigan, USA.

- Participants: Antoine Deleforge, Emeline Perthame and Florence Forbes
- Partner: University of Michigan, Ann Arbor, USA
- Contact: Florence Forbes
- Publications: Inverse regression approach to robust nonlinear high-to-low dimensional mapping - High-Dimensional Regression with Gaussian Mixtures and Partially-Latent Response Variables
- URL: https://cran.r-project.org/web/packages/xLLiM/index.html

6.4. MMST

Mixtures of Multiple Scaled Student T distributions
KEYWORDS: Health - Statistics - Brain MRI - Medical imaging - Robust clustering

SCIENTIFIC DESCRIPTION: A new family of multivariate heavy-tailed distributions that allow variable marginal amounts of tailweight is proposed and implemented. The originality comes from introducing multidimensional instead of univariate scale variables for the mixture of scaled Gaussian family of distributions. In contrast to most existing approaches, the derived distributions can account for a variety of shapes and have a simple tractable form with a closed-form probability density function whatever the dimension. We provide maximum likelihood estimation of the parameters and illustrate their modelling flexibility.
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. Recent additions include a Markov random field implementation to account for spatial dependencies between observations, and a Bayesian implementation that can be used to select the number of mixture components automatically.

RELEASE FUNCTIONAL DESCRIPTION: Recent additions include a Markov random field implementation to account for spatial dependencies between observations, and a Bayesian implementation that can be used to select the number of mixture components automatically.
NEWS OF THE YEAR: Recent additions include a Markov random field implementation to account for spatial dependencies between observations, and a Bayesian implementation that can be used to select the number of mixture components automatically.

- Participants: Alexis Arnaud, Darren Wraith, Florence Forbes, Steven Quinito Masnada and Stéphane Despréaux
- Partner: Institut des Neurosciences Grenoble
- Contact: Florence Forbes
- Publications: A new family of multivariate heavy-tailed distributions with variable marginal amounts of tailweights: Application to robust clustering - Fully Automatic Lesion Localization and Characterization: Application to Brain Tumors Using Multiparametric Quantitative MRI Data
- URL: https://team.inria.fr/mistis/software/

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 Tesselations) on other visualisation problems, such as clustering.

- Participants: Bhargav Srinivasa Desikan and Benjamin Guedj
- Contact: Benjamin Guedj
- Publication: Pycobra: A Python Toolbox for Ensemble Learning and Visualisation
- 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. MixAll

Clustering using Mixture Models
KEYWORDS: Clustering - Clustering package - Generative Models
FUNCTIONAL DESCRIPTION: MixAll is a model-based clustering package for modelling mixed data sets. It has been engineered around the idea of easy and quick integration of any kind of mixture models for any kind of data, under the conditional independence assumption. Currently five models (Gaussian mixtures, categorical mixtures, Poisson mixtures, Gamma mixtures and kernel mixtures) are implemented. MixAll has the ability to natively manage completely missing values when assumed as random. MixAll is used as an R package, but its internals are coded in C++ as part of the STK++ library (www.stkpp.org) for faster computation.

- Participant: Serge Iovleff
- Partner: Université Lille 1
- Contact: Serge Iovleff
- URL: https://cran.r-project.org/web/packages/MixAll/

6.9. simerge

Statistical Inference for the Management of Extrem Risks, Genetics and Global epidemiology
KEYWORD: Biclustering
FUNCTIONAL DESCRIPTION: Allows to perform Co-Clustering on binary (Bernoulli) and counting variables (Poisson) using co-variables.

- Partner: Inria
- Contact: Serge Iovleff

6.10. Platforms

6.10.1. 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

6. New Software and Platforms

6.1. COCO

COmparing Continuous Optimizers
KEYWORDS: Benchmarking - Numerical optimization - Black-box optimization - Stochastic optimization
SCIENTIFIC DESCRIPTION: COmparing Continuous Optimisers (COCO) is a tool for benchmarking algorithms for black-box optimisation. COCO facilitates systematic experimentation in the field of continuous optimization. COCO provides: (1) an experimental framework for testing the algorithms, (2) post-processing facilities for generating publication quality figures and tables, (3) LaTeX templates for scientific articles and HTML overview pages which present the figures and tables.

The COCO software is composed of two parts: (i) an interface available in different programming languages (C/C++, Java, Matlab/Octave, Python, external support for R) which allows to run and log experiments on several function test suites (unbounded noisy and noiseless single-objective functions, unbounded noiseless multiobjective problems, constrained problems) are provided (ii) a Python tool for generating figures and tables that can be looked at in every web browser and that can be used in the provided LaTeX templates to write scientific papers.
FUNCTIONAL DESCRIPTION: The Coco platform aims at supporting the numerical benchmarking of blackbox optimization algorithms in continuous domains. Benchmarking is a vital part of algorithm engineering and a necessary path to recommend algorithms for practical applications. The Coco platform releases algorithm developers and practitioners alike from (re-)writing test functions, logging, and plotting facilities by providing an easy-to-handle interface in several programming languages. The Coco platform has been developed since 2007 and has been used extensively within the "Blackbox Optimization Benchmarking (BBOB)" workshop series since 2009. Overall, 160+ algorithms and algorithm variants by contributors from all over the world have been benchmarked on the platform's three supported test suites so far. The most recent extension towards bi-objective problems has been used for the BBOB-2016 workshop at GECCO and we are currently developing new test suites around large-scale and constrained optimization.

- Participants: Anne Auger, Asma Atamna, Dejan Tusar, Dimo Brockhoff, Marc Schoenauer, Nikolaus Hansen, Ouassim Ait Elhara, Raymond Ros, Tea Tusar, Thanh-Do Tran and Umut Batu
- Partners: TU Dortmund University - Charles University Prague - Jozef Stefan Institute (JSI)
- Contact: Dimo Brockhoff
- URL: https://github.com/numbbo/coco

6.2. CMA-ES

Covariance Matrix Adaptation Evolution Strategy
KEYWORDS: Numerical optimization - Black-box optimization - Stochastic optimization
SCIENTIFIC DESCRIPTION: The CMA-ES is considered as state-of-the-art in evolutionary computation and has been adopted as one of the standard tools for continuous optimisation in many (probably hundreds of) research labs and industrial environments around the world. The CMA-ES is typically applied to unconstrained or bounded constraint optimization problems, and search space dimensions between three and a hundred. The method should be applied, if derivative based methods, e.g. quasi-Newton BFGS or conjugate gradient, (supposedly) fail due to a rugged search landscape (e.g. discontinuities, sharp bends or ridges, noise, local optima, outliers). If second order derivative based methods are successful, they are usually faster than the CMA-ES: on purely convex-quadratic functions, f(x)=xTHx, BFGS (Matlabs function fminunc) is typically faster by a factor of about ten (in terms of number of objective function evaluations needed to reach a target function value, assuming that gradients are not available). On the most simple quadratic function f(x)=‖x‖2=xTx BFGS is faster by a factor of about 30.

FUNCTIONAL DESCRIPTION: The CMA-ES is an evolutionary algorithm for difficult non-linear non-convex black-box optimisation problems in continuous domain.

- Participant: Nikolaus Hansen
- Contact: Nikolaus Hansen
- URL: http://cma.gforge.inria.fr/cmaes_sourcecode_page.html

6.3. Platforms

6.3.1. New developments around COCO

There were two public releases of the COCO software this year including quite some new features that have also been used for the Blackbox Optimization Benchmarking workshop (BBOB) which was held in Kyoto, Japan during GECCO-2019.

The most important new features are updated, streamlined plots, a Python 3 compatible postprocessing module with a corresponding restructuring of the postprocessing code, the support for zip files in the postprocessing, a simplified example experiment script for beginners and a non-anytime example experiment for benchmarking budget-dependent algorithms, improved coverage of the continuous integration testing via CircleCI and AppVeyor, and finally and most-important from a practical perspective an archive with automatized download from all 200+ algorithm data sets available in the COCO data archive. Of these, 17 algorithm data sets have been made newly available in 2018 with four scientific papers being presented at the BBOB-2019 workshop.

In the background, there have been additional (preparational) activities, in particular due to the two Inria ADT projects “COCOpysuites” and “COCOpost”. The “COCOpysuites” project aimed at a rewriting of the experimental part of COCO in python to allow for an easier development, testing, and implementation of new test suites. The “COCOpost” project aimed at a complete rewrite of the python postprocessing with a focus on new, interactive plots and a clearer structure for improved maintenance. In addition, new test suites have been developed and implemented for large-scale, constrained, multiobjective, and mixed-integer optimization. All those extensions will be made available step-by-step to the scientific community after proper alpha- and beta-testing in the coming planned releases.

6.3.2. Developments within the CMA-ES library

The `pycma` library has not seen major changes, but overall 39 commits pushed for maintenance, bug-fixes and smaller improvements (roughly 1000 lines of code). An as of yet unpublished development has been the modularization of the data logger. A surrogate fitness model module with 969 lines of code has been developed and is already operative but has also not yet been released.

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, Francois Vanderbeck, Halil Sen, Issam Tahiri, Michael Poss, Pierre Pesneau, Romain Leguay and Ruslan Sadykov
- Partners: Université de Bordeaux - CNRS - IPB - Universidade Federal Fluminense
- Contact: Francois Vanderbeck
- URL: https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod

6.2. WineryPlanning

- Participants: Agnes Le Roux, Alexis Toullat, Francois Vanderbeck, Issam Tahiri and Ruslan Sadykov
- Contact: Francois 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 paradign) 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: Francois Vanderbeck, Guillaume Marques, Issam Tahiri and Ruslan Sadykov
- Contact: Issam Tahiri

6.4. pmtool

KEYWORDS: Scheduling - Task scheduling - StarPU - Heterogeneity - GPGPU - Performance analysis
FUNCTIONAL DESCRIPTION: Analyse post-mortem the behavior of StarPU applications. Provide lower bounds on makespan. Study the performance of different schedulers in a simple context. Provide implementations of many scheduling algorithms from the literature

NEWS OF THE YEAR: Included many new algorithms, in particular online algorithms Better integration with StarPU by accepting .rec files as input

- Participant: Lionel Eyraud-Dubois
- Contact: Lionel Eyraud-Dubois
- Publications: Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs - Fast Approximation Algorithms for Task-Based Runtime Systems
- URL: https://gitlab.inria.fr/eyrauddu/pmtool

6.5. Platforms

6.5.1. Bapcod

We have developed a stabilized Benders' decomposition in our generic library BapCod. This allowed to produce state-of-the-art results for an energy production planning.

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: Christophe Biernacki
- URL: https://massiccc.lille.inria.fr

5.3. Mixmod

Many-purpose software for data mining and statistical learning
KEYWORDS: Data mining - Classification - Mixed data - Data modeling - 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 Langrognet, Gérard Govaert, Gilles Celeux, Remi Lebret and Serge Iovleff
- Partners: CNRS - Université Lille 1 - LIFL - Laboratoire Paul Painlevé - HEUDIASYC - LMB
- Contact: Gilles Celeux
- URL: http://www.mixmod.org

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

6.5. DPPy

Sampling Determinantal Point Processes with Python
KEYWORD: Determinantal point processes
FUNCTIONAL DESCRIPTION: Determinantal point processes (DPPs) are specific probability distributions over clouds of points that are used as models and computational tools across physics, probability, statistics, and more recently machine learning. Sampling from DPPs is nontrivial and therefore we present. DPPy, a Python toolbox that gathers known exact and approximate sampling algorithms. The project is hosted on GitHub and equipped with an extensive documentation.

- Contact: Guillaume Gautier
- URL: https://github.com/guilgautier/DPPy/

6.6. SMPyBandits

Open-Source Python package for Single- and Multi-Players multi-armed Bandits algorithms.
KEYWORD: Machine learning
FUNCTIONAL DESCRIPTION: The library contains the implementation of many single-player mutli-armed bandit algorithms as well as the implementation of all the state-of-the-art multi-player algorithms.

- Contact: Lilian Besson

SIERRA Project-Team

6. New Software and Platforms

6.1. 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

6.2. 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.

- Participants: Jean-Baptiste Alayrac, Josef Sivic, Ivan Laptev and Simon Lacoste-Julien
- Contact: Jean-Baptiste Alayrac
- Publication: Joint Discovery of Object States and Manipulation Actions
- URL: https://github.com/jalayrac/object-states-action

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.

(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 (Findable, Accessible, Interoperable, and Reusable - Wilkinson, M., Nature Scientific Data 2016) principles through a user-centric approach.

- 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 anlysis 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, Cartolabe provides the user with a map of the thematics, authors and articles . 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

- Partners: LRI - Laboratoire de Recherche en Informatique - CNRS
- Contact: Philippe Caillou
- URL: http://www.cartolabe.fr/

CQFD Project-Team

5. New Software and Platforms

5.1. 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

5.2. 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

5.3. 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
- URL: https://cran.r-project.org/web/packages/QuantifQuantile/index.html

MATHRISK Project-Team

6. New Software and Platforms

6.1. 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, Jérôme Lelong and Bernard Lapeyre
- Partners: Inria - Ecole des Ponts ParisTech - Université Paris-Est
- Contact: Agnes Sulem
- URL: http://www.premia.fr

6.2. Platforms

6.2.1. Development of the quantitative platform Premia in 2018

Premia 20 has been delivered to the Consortium Premia on March 12th. It contains the following new algorithms :

6.2.1.1. Optimal Trade Execution, Risk Management, Insurance

- Optimal Execution Under Jump Models For Uncertain Price Impact. S.Moazeni, T.F.Coleman, Y.Li
  The Journal of Computational Finance. Vol. 18, Issue 3, 2015.
- Nested Monte Carlo for Risk Margin computation. L.A. Abbas-Turki, S.Crepey, B.Diallo.
- Efficient Estimation of Sensitivities for Counterparty Credit Risk with the Finite Difference Monte-Carlo Method. C. S.L. de Graaf, D.Kandhai, P.M.A.Sloot.
  The Journal of Computational Finance, Volume 21, Issue 1, 2017.
- Nested Simulation in Portfolio Risk Measurement. M.B.Gordy, S.Juneja
  Management Science, Vol 56, Issue 10, 2010
- Spectral methods for the calculation of risk measures for variable annuity guaranteed benefits. R. Feng, H.W. Volkmer
  ASTIN Bull., 44(3), 2014
- Fast computation of risk measures for variable annuities with additional earnings by conditional moment matching. N. Privault X.Wei
  ASTIN Bull., 48(1):171–196, 2018.

6.2.1.2. Equity Derivatives

- Pricing under Rough volatility. C. Bayer, P.Friz, J. Gatheral
  Quantitative Finance, Vol. 16, No. 6, 887-904, 2016.
- Hybrid scheme for Brownian semistationary processes. M. Bennedsen, A. Lunde, M.S.Pakkanen
  Finance and Stochastics 21(4), 931–965, 2017.
- Antithetic multilevel Monte Carlo estimation for multi-dimensional SDEs without Lévy area simulation. M. B. Giles and L. Szpruch
  The Annals of Applied Probability, Vol. 24, No. 4, 2014
- Fourier transform algorithms for pricing and hedging discretely sampled exotic variance products and volatility derivatives under additive processes. W. Zheng and Y. K. Kwok
  The Journal of Computational Finance, Volume 18, Issue 2, 2014.
- Efficient Solution of Backward Jump-Diffusion PIDEs with Splitting and Matrix Exponentials. A.Iktin
  The Journal of Computational Finance, Volume 19, Issue 3, 2016
- High-Order Splitting Methods for Forward PDEs and PIDEs. A.Iktin
  International Journal of Theoretical and Applied Finance, 18(5), 2015
- Pricing Bullet option on local volatility model using GPU L.A. Abbas-Turki
- Pricing Bermudan Options via Multilevel Approximation Methods. D. Belomestny, F. Dickmann, T.Nagapetyan.
  Siam J. Financial Math., Volume 6, 2015.
- Pricing CIR yield options by conditional moment matching. A. Prayoga N. Privault
  Asia-Pacific Financial Markets, 24:19–38, 2017

We benefit from the help of the engineer Pierre-Guillaume Raverdy.

SIMSMART Team (section vide)

TOSCA Project-Team (section vide)