RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2019

Section Software

NUMERICAL SCHEMES AND SIMULATIONS

OPTIMIZATION AND CONTROL OF DYNAMIC SYSTEMS

OPTIMIZATION, MACHINE LEARNING AND STATISTICAL METHODS

<p style="color:red; text-align:center;">**ACUMES Project-Team**</p>

5. New Software and Platforms

5.1. MGDA

Multiple Gradient Descent Algorithm

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

SCIENTIFIC DESCRIPTION: The software relies upon a basic MGDA tool which permits to calculate a descent direction common to an arbitrary set of cost functions whose gradients at a computational point are provided by the user, as long as a solution exists, that is, with the exclusion of a Pareto-stationarity situation.

More specifically, the basic software computes a vector d whose scalar product with each of the given gradients (or directional derivative) is positive. 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.

This basic tool admits the following extensions: - constrained multi-objective optimization - prioritized multi-objective optimization - stochastic multi-objective optimization.

FUNCTIONAL DESCRIPTION: Chapter 1: Basic MGDA tool Software to compute a descent direction common to an arbitrary set of cost functions whose gradients are provided in situations other than Pareto stationarity.

Chapter 2: Directions for solving a constrained problem Guidelines and examples are provided according the Inria research report 9007 for solving constrained problems by a quasi-Riemannian approach and the basic MGDA tool.

Chapter 3: Tool for prioritized optimization Software permitting to solve a multi-objective optimization problem in which the cost functions are defined by two subsets: - a primary subset of cost functions subject to constraints for which a Pareto optimal point is provided by the user (after using the previous tool or any other multiobjective method, possibly an evolutionary algorithm) - a secondary subset of cost functions to be reduced while maintaining quasi Pareto optimality of the first set. Procedures defining the cost and constraint functions, and a small set of numerical parameters are uploaded to the platform by an external user. The site returns an archive containing datafiles of results including graphics automatically generated.

Chapter 4: Stochastic MGDA Information and bibliographic references about SMGDA, an extension of MGDA applicable to certain stochastic formulations.

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
- Publications: Revision of the Multiple-Gradient Descent Algorithm (MGDA) by Hierarchical Orthogonalization - Parametric optimization of pulsating jets in unsteady flow by Multiple-Gradient Descent Algorithm (MGDA) - A quasi-Riemannian approach to constrained optimization - Platform for prioritized multi-objective optimization by metamodel-assisted Nash games - Direct and adaptive approaches to multi-objective optimization
- URL: http://mgda.inria.fr

5.2. Igloo

Iso-Geometric anaLysis using discOntinuOus galerkin methods

KEYWORDS: Numerical simulations - Isogeometric analysis

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

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

- Author: Régis Duvigneau
- Contact: Régis Duvigneau

5.3. BuildingSmart

BuildingSmart interactive visualization

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

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

FUNCTIONAL DESCRIPTION: The main task of the project is to study and develop solutions dedicated to interactive visualisation of building performances (heat, structural) in relation to the Building Information Modeling BIM framework, using 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 2019, the following points were addressed in AeroSol

*Update, documentation, and wiki for the test case

*exact solution of Riemann problem and exact Godunov solver

*Development of Droplet model, and of a Baer and Nunziato diphasic model.

*Beginning of implementation of eddy viscosity models (k-epsilon, Spalart-Almarras) turbulence models.

*Add the possibility of mesh dependent data (for example, a flow computed by AeroSol with the Euler system) for being used as input for another model (e.g. advection of droplets within this flow). This feature is used also for wall distance for turbulent models.

*Penalization problems, with single core mesh adaptation was merged in the master branch.

*Improvements of PETSc usage: possibility of solving linear problems that are not of size nvar, usage of MUMPS LU solver through PETSc.

*Interfacing with SLEPc for solving eigenvalues and eigenvectors problems.

*High order visualization based on GMSH.

*Beginning of interfacing with PARMMG for parallel mesh adaptation.

*Clean of warning, error messages, etc...

- Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, Héloïse Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung and Enrique Gutierrez Alvarez
- Partner: BRGM
- Contact: Vincent Perrier

<p style="text-align:center">**CARDAMOM Project-Team**</p>

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 2019, the following points were addressed in AeroSol

*Update, documentation, and wiki for the test case

*exact solution of Riemann problem and exact Godunov solver

*Development of Droplet model, and of a Baer and Nunziato diphasic model.

*Beginning of implementation of eddy viscosity models (k-epsilon, Spalart-Almarras) turbulence models.

*Add the possibility of mesh dependent data (for example, a flow computed by AeroSol with the Euler system) for being used as input for another model (e.g. advection of droplets within this flow). This feature is used also for wall distance for turbulent models.

*Penalization problems, with single core mesh adaptation was merged in the master branch.

*Improvements of PETSc usage: possibility of solving linear problems that are not of size nvar, usage of MUMPS LU solver through PETSc.

*Interfacing with SLEPc for solving eigenvalues and eigenvectors problems.

*High order visualization based on GMSH.

*Beginning of interfacing with PARMMG for parallel mesh adaptation.

*Clean of warning, error messages, etc...

- Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, Héloïse Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung and Enrique Gutierrez Alvarez
- Partner: BRGM
- Contact: Vincent Perrier
- URL: https://team.inria.fr/cardamom/aerosol/

6.2. Mmg

Mmg Plateform

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

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

6.4. 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 Giulia Bellezza
- Partner: LCTS (UMR 5801)
- Contact: Mario Ricchiuto

6.5. 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: Maria Kazolea and Mario Ricchiuto
- Contact: Mario Ricchiuto
- URL: https://team.inria.fr/cardamom/slows-shallow-water-flows/

6.6. 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: Technical University of Crete
- Contact: Maria Kazolea

6.7. 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: Leo Nouveau, Luca Arpaia, Mario Ricchiuto and Luca Cirrottola
- Contact: Algiane Froehly

6.8. ParMmg

KEYWORDS: 3D - Mesh adaptation - Anisotropic - Isotropic - Isovalue discretization - Distributed Applications - MPI communication

FUNCTIONAL DESCRIPTION: The ParMmg software build parallel (MPI based) mesh adaptation capabilities on top of the sequential open-source remesher Mmg, iteratively called over sub-meshes of the initial mesh.

ParMmg is available: - through command line , - in library mode using the dedicated API.

RELEASE FUNCTIONAL DESCRIPTION: The version 1.2 of ParMmg provide 3D volume mesh adaptation with constrained surface.

It adds to the previous release: - Mesh repartitioning through parallel interface displacement , - Support for Scotch renumeration.

- Participants: Algiane Froehly and Luca Cirrottola
- Partners: FUI Icarus - ExaQUte
- Contact: Algiane Froehly
- URL: https://mmgtools.org

DEFI Project-Team (section vide)

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 the so-called Activity analysis, Adjoint Liveness analysis, and TBR analysis.

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++ (using Clang-LLVM) - Preliminary work, including refactoring, in view of future Open-Source distribution

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

<p style="text-align:center">**ELAN Project-Team**</p>

6. New Software and Platforms

6.1. 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). The Argus-distribution code was awarded in 2019 the [Graphics Replicability stamp](http://www.replicabilitystamp.org/), which acknowledges its reproducibility.

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

6.2. Feel++

KEYWORDS: High order finite elements - Discontinuous Galerkin - High-Performance Computing

FUNCTIONAL DESCRIPTION: Feel++ is a high-performance C++ library for the resolution of general variational formulations, including continuous and discontinuous Galerkin methods, finite element or spectral element methods, reduced basis formulations, etc. It features a high-level domain specific embedded language (DSEL) for Galerkin methods, space dimension-agnostic computation kernels and seamless and automatic parallelism. It also includes applicative toolboxes to solve physics problems in fluid mechanics, solid mechanics, thermal conduction, and the corresponding multi-physics coupling.

- Partners: Université de Strasbourg - UGA - Inria
- Contact: Thibaut Metivet
- URL: http://www.feelpp.org

GAMMA Project-Team

3. New Software and Platforms

3.1. Metrix

Metrix: Error Estimates and Mesh Control for Anisotropic Mesh Adaptation

KEYWORDS: Meshing - Metric - Metric fields

FUNCTIONAL DESCRIPTION: Metrix is a software that provides by various ways metric to govern the mesh generation. Generally, these metrics are constructed from error estimates (a priori or a posteriori) applied to the numerical solution. Metrix computes metric fields from scalar solutions by means of several error estimates: interpolation error, iso-lines error estimate, interface error estimate and goal oriented error estimate. It also contains several modules that handle meshes and metrics. For instance, it extracts the metric associated with a given mesh and it performs some metric operations such as: metric gradation and metric intersection.

- Participants: Adrien Loseille and Frédéric Alauzet
- Contact: Frédéric Alauzet
- URL: https://www.rocq.inria.fr/gamma/Frederic.Alauzet/code_eng.html

MATHERIALS Project-Team

5. New Software and Platforms

5.1. DFTK

KEYWORDS: Molecular simulation - Quantum chemistry - Materials

FUNCTIONAL DESCRIPTION: DFTK, short for the density-functional toolkit, is a Julia library implementing plane-wave density functional theory for the simulation of the electronic structure of molecules and materials. It aims at providing a simple platform for experimentation and algorithm development for scientists of different backgrounds.

- Contact: Antoine Levitt
- URL: http://dftk.org

5.2. gen.parRep

KEYWORDS: Molecular simulation - MPI - HPC - C++

SCIENTIFIC DESCRIPTION: Metastability is one of the major encountered obstacle when performing long molecular dynamics simulations, and many methods were developed to address this challenge. The "Parallel Replica" (ParRep) dynamics is known for allowing to simulate very long trajectories of metastable Langevin dynamics in the materials science community, but it relies on assumptions that can hardly be transposed to the world of biochemical simulations. The later developed "Generalized ParRep" variant solves those issues, but it was not applied to significant systems of interest so far.

In a recent article article, we presented the program gen.parRep, the first publicly available implementation of the Generalized Parallel Replica method (BSD 3-Clause license), targeting frequently encountered metastable biochemical systems, such as conformational equilibria or dissociation of protein-ligand complexes. It was shown that the resulting C++ implementation exhibits a strong linear scalability, providing up to 70 % of the maximum possible speedup on several hundreds of CPUs.

FUNCTIONAL DESCRIPTION: gen.parRep is the first publicly available implementation of the Generalized Parallel Replica method (BSD 3-Clause license), targeting frequently encountered metastable biochemical systems, such as conformational equilibria or dissociation of protein-ligand complexes.

It was shown (https://hal.archives-ouvertes.fr/hal-01832823) that the resulting C++/MPI implementation exhibits a strong linear scalability, providing up to 70 % of the maximum possible speedup on several hundreds of CPUs.

RELEASE FUNCTIONAL DESCRIPTION: The software was modified in order to allow reproducibility in some cases (the limiting factor is OpenMM which does not always provides deterministic output even when using the same seeds (!), see http://docs.openmm.org/latest/userguide/library.html#determinism).

The main executable now has 2 more command line options, '–inp-seeds [fname]' or '–out-seeds [fname]' for respectively loading seeds or writing seeds from/to a unique binary file. See rand.hpp/rand.cpp, od the Doxygen doc for more details.

These modifications now allow Continuous Integration (CI) on the infrastructure provided by Inria : in mol/ci a small test case will be executed at each commit to the repository and compared to reference results.

The two other minor modifications concern the Lua scripts:

"get_minimised_energy_crdvels" was added to the set of functions that the user can call from the Lua script : it simply combines in one call what "get_minimised_energy" and "get_minimised_crdvels" already provided.

a extra optional parameter is available for the "simulation" parameters block when "simulation.algorithm" is "PARREP_FV" , this parameter is "simulation.minAccumulatedObs" : it will enforce that at least minAccumulatedObs observations of an observable have already been accumulated before the convergence test is performed , this may be useful if there is a risk of early pseudo-convergence for some of the observables when only a few samples have been accumulated.

Download sources:

https://gitlab.inria.fr/parallel-replica/gen.parRep/tags/v1.2.0

or

https://github.com/FHedin/gen.parRep/releases/tag/v1.2.0

NEWS OF THE YEAR: Corresponding publication : https://hal.archives-ouvertes.fr/hal-01832823

- Participants: Florent Hedin and Tony Lelièvre
- Partner: Ecole des Ponts ParisTech
- Contact: Florent Hedin
- Publication: gen.parRep: a first implementation of the Generalized Parallel Replica dynamics for the long time simulation of metastable biochemical systems
- URL: https://gitlab.inria.fr/parallel-replica/gen.parRep

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.

- Authors: Alexia De Brauer, Florian Bernard, Yannick Gorsse, Thomas Milcent and Angelo Iollo
- Partners: CNRS - Université Bordeaux 1
- Contact: Florian Bernard
- URL: https://gforge.inria.fr/projects/cocoflow

6.2. KOPPA

Kinetic Octree Parallel PolyAtomic

KEYWORDS: C++ - 3D - MPI

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
- Partners: Université de Bordeaux - INP Bordeaux - CNRS
- Contact: Angelo Iollo
- 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
- Partner: Université de Bordeaux
- 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 Team (section vide)

MINGUS Project-Team

5. New Software and Platforms

5.1. 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/

<p style="text-align:center">**MOKAPLAN Project-Team**</p>

4. New Software and Platforms

4.1. 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/

4.2. 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/

<p align="center" style="color:red">NACHOS Project-Team</p>

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 Gobé 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.

- Authors: Ludovic Moya and Alexis Gobé
- Contact: Stéphane Lanteri
- URL: http://www-sop.inria.fr/nachos/index.php/Software/HORSE

<p style="text-align:center">**NANO-D Team**</p>

5. New Software and Platforms

5.1. 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 Sergei Grudinin
- Partner: MIPT Moscow
- Contact: Sergei 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/

5.2. 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 Sergei Grudinin
- Contact: Sergei 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/

5.3. 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.

RELEASE FUNCTIONAL DESCRIPTION: Version 0.7 from 3 Sep 2018: mmCIF support added. A file can be gzipped. Version 0.8 from 30 July 2019: Checks the similarity between chains. Explicitly output when an incomplete assembly is detected as symmetric. Version 0.9 from 8 Nov 2019: Added lists of excluded chains for both PDB and CIF formats.

- Participants: Guillaume Pages and Sergei Grudinin
- Contact: Sergei 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/

5.4. 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.

RELEASE FUNCTIONAL DESCRIPTION: Version 1.0 from 6th March 2018: Added computation of P(r). Version 1.1 from 19th April 2018: Excluded solvent radii updated. Many more ions added. Version 1.2 from 24th April 2018: Added automatic identification of labile and nonlabile explicit hydrogens. Added bulk SLD option. Version 1.3 from 30th July 2018: Added initial prototype of 2D dcattering images. Version 1.4 from 1st August 2018: Added docking module. Version 2.0 from January 2019: Added flexible optimization of conformations. A bug with absolute contrast fixed. Default behaiviour of Pepsi-SAXS changed, now it reads all the hydrogen atoms if the –hyd flag is set. Otherwise, it reads only explicit hydrogens on non-standard residues. Version 2.1 from February 2019: First implimentation of the multi-structure fitting.

- Participant: Sergei Grudinin
- Partner: MIPT Moscow
- Contact: Sergei 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/

5.5. 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 nonlinear normal mode analysis of macromolecules.

RELEASE FUNCTIONAL DESCRIPTION: Version 1.2 from January 2019: Exclusion interaction list added. Version 1.3 from April 2019: Sequence and structural alignment fixed thanks to Guillaume Pages. More advanced iterative structural alignment added. Version 1.4 from June 2019: Firt version of domain identification added. Please use the "–nDomains" option Version 1.5 from July 2019: Rigid block format updated. JSON and Text output formats added. Version 1.6 from December 2019: Added initial Voronota support.

- Participants: Sergei Grudinin and Alexandre Hoffmann
- Contact: Sergei 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/

5.6. 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 Sergei Grudinin
- Contact: Sergei Grudinin
- Publication: Smooth orientation-dependent scoring function for coarse-grained protein quality assessment
- URL: https://team.inria.fr/nano-d/software/sbrod/

5.7. 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 Sergei Grudinin
- Contact: Sergei Grudinin
- Publication: Protein model quality assessment using 3D oriented convolutional neural networks
- URL: https://team.inria.fr/nano-d/software/ornate/

POEMS Project-Team

5. New Software and Platforms

5.1. COFFEE

KEYWORDS: Numerical simulations - Wave propagation - Boundary element method

FUNCTIONAL DESCRIPTION: COFFEE is an adapted fast BEM solver to model acoustic and elastic wave propagation (full implementation in Fortran 90). The 3-D acoustic or elastodynamic equations are solved with the boundary element method accelerated by the multi-level fast multipole method or a hierarchical-matrices based representation of the system matrix. The fundamental solutions for the infinite space are used in this implementation. A boundary element-boundary element coupling strategy is also implemented so multi-region problems (strata inside a valley for example) can be solved. In order to accelerate the convergence of the iterative solver, various analytic or algebraic preconditioners are available. Finally, an anisotropic mesh adaptation strategy is used to further reduce the computational times.

- Contact: Stéphanie Chaillat

5.2. XLiFE++

KEYWORDS: Numerical simulations - Finite element modelling - Boundary element method

FUNCTIONAL DESCRIPTION: XLiFE++ is an FEM-BEM C++ code developed by POEMS laboratory and IRMAR laboratory, that can solve 1D/2D/3D, scalar/vector, transient/stationary/harmonic problems. Description: https://uma.ensta-paristech.fr/soft/XLiFE++/

- Contact: Eric Lunéville

6. New Software and Platforms

6.1. Platforms

6.1.1. Platform NS2DDV-M

NS2DDV-M [42] is a Matlab code, developed by C. Calgaro, 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 embeds parallel computation facilities, and is freely distributed, to allow for easy comparisons with concurrent codes on benchmark test-cases, and to promote new collaborations in the domain.

6.1.2. Platform KinDiff

KinDiff consists in a Python library and a Jupyter Notebook. It has been developed by M. Bessemoulin-Chatard (CNRS and Université de Nantes), M. Herda, and T. Rey. The KinDiff code approximates the solutions to the kinetic Fokker–Planck and linear BGK equations in a unidimensional periodic domain in space and a symmetric bounded unidimensional domain in velocity. Its outputs are the discretization of the distribution function in the phase space as well as the moments, along with some visualizations of these quantities. Kinetic equations display asymptotic behaviors such as return to equilibrium in large time, or convergence towards macroscopic equations in the diffusive limit. The finite volume method implemented within KinDiff reproduces these asymptotics at the discrete level. The presentation and numerical analysis of the scheme is available in the article [17]. The code is available at gitlab.com/thoma.rey/FV_HipoDiff.

CAGE Project-Team

5. New Software and Platforms

5.1. 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 Andréani, Jinyan Liu, Joseph Frédéric Bonnans and Pierre Martinon
- Contact: Pierre Martinon
- URL: http://bocop.org

5.2. 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

<p align="center">**COMMANDS Project-Team**</p>

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 Andréani, 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 (section vide)

FACTAS Project-Team (section vide)

<p align="center" style="color:red">I4S Project-Team</p>

5. New Software and Platforms

5.1. Platforms

5.1.1. Pegase

PEGASE is the wireless platform developed by the team. The milestones for the PEGASE platfom in 2019 are

- finalization of the PEGASE3 hardware and software platform: SDK, decoding FPGA-based GPS frames,
- capacity (demonstrated during work with CEA Lost) of synchronous transmission / reception and ultrasonic wave phase.
- Writing documentation associated with the platform (User Guide ...).
- Start of the valuation process.

A prototype for modal analysis with several PEGASE platforms was developed. To obtain detailed modal information of large and very large structures, many sensors would be required to cover the geometry of the structure with a reasonable accuracy. However, when only a limited amount of sensors is available, large structures can be measured in several sensor setups, where some sensors remain fixed and some are moved between different measurement setups. With the sensors connected to different wireless platforms, the synchronous acquisition of data is required. A solution of data acquisition synchronization, as well as signal processing for merging the information taking into account the change of sensor positions and environmental variability has been developed and presented at IWSHM [31].

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 developed to solve optimal control problems by a combination of Hamiltonian et path following methods. Hampath includes shooting and computation of conjugate points. It is an evolution of the software cotcot (apo.enseeiht.fr/cotcot). 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 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, Remi 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/

QUANTIC Project-Team (section vide)

<p style="text-align:center;color:red;">SPHINX Project-Team</p>

6. New Software and Platforms

6.1. GetDDM

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

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

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

6.2. 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/

<p align="center" style="color:red">TRIPOP Project-Team</p>

5. New Software and Platforms

5.1. 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/

<p style="text-align:center">**TROPICAL Project-Team**</p>

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

NEWS OF THE YEAR: Coq-Polyhedra now provides most of the basic operations on polyhedra. They are expressed on a quotient type that avoids reasoning with particular inequality representations. They include : * the construction of elementary polyhedra (half-spaces, hyperplanes, affine spaces, orthants, simplices, etc) * basic operations such as intersection, projection (thanks to the formalization of the Fourier-Motzkin algorithm), image under linear functions, computations of convex hulls, finitely generated cones, etc. * computation of affine hulls of polyhedra, as well as their dimension

Thanks to this, we have made huge progress on the formalization of the combinatorics of polyhedra. The poset of faces, as well as its fundamental properties (lattice, gradedness, atomicity and co-atomicity, etc) are now formalized. The manipulation of the faces is based on an extensive use of canonical structures, that allows to get the most appropriate inequality representations for reasoning. In this way, we arrive at very concise and elegant proofs, closer to the pen-and-paper ones.

- Participants: Xavier Allamigeon, Vasileios Charisopoulos, Ricardo Katz and Pierre-Yves Strub
- Partners: CIFASIS - Ecole Polytechnique
- 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

6.2. EmergencyEval

KEYWORDS: Dynamic Analysis - Simulation - Ocaml - Emergency - Firefighters - Police

SCIENTIFIC DESCRIPTION: This software aims at enabling the definition of a Petri network execution semantic, as well as the instanciation and execution of said network using the aforedefined semantic.

The heart of the project dwells in its kernel which operates the step-by-step execution of the network, obeying rules provided by an oracle. This user-defined and separated oracle computes the information necessary to the kernel for building the next state using the current state. The base of our software is the framework for the instanciation and execution of Petri nets, without making assumptions regarding the semantic.

In the context of the study of the dynamics of emergency call centers, a second part of this software is the definition and implementation of the semantic of call centers modelized as Petri nets, and more specifically timed prioritized Petri nets. A module interoperating with the kernel enables to include all the operational specificities of call centers (urgency level, discriminating between operators and callers ...) while guaranteeing the genericity of the kernal which embeds the Petri net formalism as such.

FUNCTIONAL DESCRIPTION: In order to enable the quantitative study of the throughput of calls managed by emergency center calls and the assesment of various organisationnal configurations considered by the stakeholders (firefighters, police, medical emergency service of the 75, 92, 93 and 94 French departments), this software modelizes their behaviours by resorting to extensions of the Petri net formalism. Given a call transfer protocol in a call center, which corresponds to a topology and an execution semantic of a Petri net, the software generates a set of entering calls in accord with the empirically observed statistic ditributions (share of very urgent calls, conversation length), then simulates its management by the operators with respect to the defined protocol. Transitional regimes phenomenons (peak load, support) which are not yet handled by mathematical analysis could therefore be studied. The ouput of the software is a log file which is an execution trace of the simulation featuring extensive information in order to enable the analysis of the data for providing simulation-based insights for decision makers.

The software relies on a Petri net simulation kernel designed to be as modular and adaptable as possible, fit for simulating other Petri-net related phenomenons, even if their semantic differ greatly.

- Participants: Baptiste Colin and Xavier Allamigeon
- Contact: Baptiste Colin

VALSE Project-Team

6. New Software and Platforms

6.1. Platforms

6.1.1. ControlHub

ControlHub is the platform for the rapid prototyping of control algorithms of cyber-physical systems. It allows the End-User to have a remote access to real experimental setups in order to validate mathematical control and estimation algorithms.

<h1 style="text-align:center; color:red;">BONUS Project-Team</h1>

6. New Software and Platforms

6.1. Platforms

6.1.1. Grid'5000 testbed: extension with storage and 10G network at Lille

Participants: Nouredine Melab [contact person], Dimitri Delabroye, Thierry Peltier [external collaborator], Lucas Nussbaum [external collaborator].

Keywords: Experimental testbed, large-scale computing, high-performance computing, GPU computing, cloud computing, big data

Functional description: Grid'5000 is a project intiated in 2003 by the French government to promote scientific research on large scale distributed systems. The project is later supported by 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 equipement. 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 mainly two storage serveurs 200TB and a 10G Internet connexion to the testbed. 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.

URL: https://www.grid5000.fr/mediawiki/index.php/Grid5000:Home

CELESTE 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.

RELEASE FUNCTIONAL DESCRIPTION: Initialization strategy enhanced

- 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

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 speech disorders. The software can train usual classifiers (SVM, random forests, etc) on these databases as well as classify new signals.

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

6.4. superres

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

KEYWORD: Multiscale

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

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

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

6.5. EdgeReconstruct

Edge Reconstruction With UPM Manifold

KEYWORDS: 2D - Fractal - Signal processing

FUNCTIONAL DESCRIPTION: EdgeReconstruct is a software that reconstructs a complex signal from the computation of most 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

6.7. Amuencha

Musical analyzer and singing training

KEYWORDS: Audio - Real-time rendering

SCIENTIFIC DESCRIPTION: The typical audio analyzer uses Fast Fourier Transforms (FFT) in order to find the frequency content. The problem with this approach is that notes follow the logarithm of the frequencies. . . while the FFT is linear in frequency. This results in a loss of precision. Even worse, the window function used for localizing the frequencies in time is often non-optimal, which increases this precision loss. Generally, nearby frequencies « bleed on » the one being analyed. Amuencha does not uses FFT. I first create a bank of filters, each centered on one frequency to analyze. These filters are complex exponentials convoluted with a Kaiser window, which support is set according to the frequency to analyze. Once these filters are applied to the signal, I use a time-frequency reassignement technique in order to exploit the complex phase of the signal. This method combines the information from nearby filters, but with a different phase, in order to restore very precisely the frequency content with the smallest possible delay.

FUNCTIONAL DESCRIPTION: Amuencha gathers notes separated by an octave along the same directions of a spiral, so that chords clearly stand out, even reversed. You can also record yourself with a microphone (in red) while playing some recording (in blue), so you can work your tuning :-)

RELEASE FUNCTIONAL DESCRIPTION: Initial version

- Author: Nicolas Brodu
- Contact: Nicolas Brodu
- URL: https://nicolas.brodu.net/programmation/amuencha/

6.8. Manzana

KEYWORDS: 2D - Image processing - Filtering

SCIENTIFIC DESCRIPTION: Software library developed in the framework of I2S-GEOSTAT innovationlab and made of high-level image processing functionalities based on sparsity and non-convex optimization.

FUNCTIONAL DESCRIPTION: Library of software in image processing: filtering, hdr, inpainting etc.

- Partner: Innovative Imaging Solutions I2S
- Contact: Hussein Yahia

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 schedule 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: Frederic 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.). It 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 Labbé

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: 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/

<h1 style="text-align:center; color:red;">MODAL Project-Team</h1>

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, Etienne Goffinet, Matthieu Marbac-Lourdelle, Quentin Grimonprez, Serge Iovleff and Vincent Kubicki
- Contact: Christophe Biernacki
- URL: https://cran.r-project.org/web/packages/RMixtComp/index.html

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.

RELEASE FUNCTIONAL DESCRIPTION: Initialization strategy enhanced

- 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.

RELEASE FUNCTIONAL DESCRIPTION: clusterPredict allow to predcit membership for a new data set using a previously estimated model

- 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. MixtComp.V4

KEYWORDS: Clustering - Statistics - Missing data - Mixed 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. Five basic models (Gaussian, Multinomial, Poisson, Weibull, NegativeBinomial) are implemented, as well as two advanced models (Functional 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.

RELEASE FUNCTIONAL DESCRIPTION: - New I/O system - Replacement of regex library - Improvement of initialization - Criteria for stopping the algorithm - Added management of partially missing data for several models - User documentation - Adding user features in R

- Participants: Christophe Biernacki, Vincent Kubicki, Matthieu Marbac-Lourdelle, Serge Iovleff, Quentin Grimonprez and Etienne Goffinet
- Partners: Université de Lille - CNRS
- Contact: Christophe Biernacki

6.11. 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

6.12. Platforms

6.12.1. 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 obtaining 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. In 2019, a new version of the MixtComp software has been developed.

RANDOPT Project-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, including the easy integration of data from benchmarking experiments of 300+ algorithm variants, (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, 300+ algorithms and algorithm variants by contributors from all over the world have been benchmarked on the platform's supported test suites so far. The most recent extension has been towards large-scale problems and was used for the BBOB-2019 workshop at the ACM-GECCO conference.

- Participants: Anne Auger, Asma Atamna, Dejan Tusar, Dimo Brockhoff, Marc Schoenauer, Nikolaus HANSEN, Ouassim Ait Elhara, Raymond Ros, Tea Tusar, Thanh-Do Tran, Umut Batu and Konstantinos Varelas
- 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, $f(x)=x^THx$, 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 $f(x)=\|x\|^2=x^Tx$ 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

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).

RELEASE FUNCTIONAL DESCRIPTION: An important update to make BaPCod compatible with VRPSolver. Correction of numerous bugs.

- 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: Ruslan Sadykov
- URL: https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod

6.2. 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

6.3. 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

<div align="center" style="color:red">**SEQUEL Project-Team**</div>

6. New Software and Platforms

6.1. gym-backgammon

Backgammon environment

KEYWORD: Artificial intelligence

FUNCTIONAL DESCRIPTION: This software program follows the openai gym API (https://gym.openai.com/), that is the interaction loop of reinforcement learning: the game is in a certain state, the agent selects an action, this action is simulated in the game, and the next state of the game as well as the return are returned to the agent. All these notions follows backgammon rules and should be understood as pertaining to the reinforcement learning vocabulary. As far as we are aware of, gym-backgammon is the only existing software of this type, and it is available in open source. Great care has been put into the debugging and the efficiency. This software program is developed in python. The inetraction is made according to a client-server model.

- Author: Alessio Della Libera
- Contact: Philippe Preux
- URL: https://github.com/dellalibera/gym-backgammon

6.2. gym-rubik

Rubik's cube environment

KEYWORD: Artificial intelligence

FUNCTIONAL DESCRIPTION: This software program follows the openai gym API (https://gym.openai.com/), that is the interaction loop of reinforcement learning: the game is in a certain state, the agent selects an action, this action is simulated in the game, and the next state of the game as well as the return are returned to the agent. All these notions follows Rubik's cube rules and should be understood as pertaining to the reinforcement learning vocabulary. Great care has been put into the debugging and the efficiency. This software program is developped in python.

- Author: Raphaël Avalos Martinez De Escobar
- Contact: Philippe Preux
- URL: https://github.com/raphaelavalos/gym-rubikscube

6.3. highway-env

An environment for autonomous driving decision-making

KEYWORDS: Generic modeling environment - Simulation - Autonomous Cars - Artificial intelligence

FUNCTIONAL DESCRIPTION: The environment is composed of several variants, each of which corresponds to driving scenes: highway, roundabout, intersection, merge, parking, etc. The road network is described by a graph, and is then populated with simulated vehicles. Vehicle kinematics follows a simple Bicycle model, and their behavior is determined by models derived from road traffic simulation literature. The ego-vehicle has access to a description of the scene through several types of observations, and its behavior is controlled through an action space, either discrete (change of lanes, of cruising speed) or continuous (accelerator pedal, steering wheel angle). The objective function to maximize is also described by the environment and may vary depending on the task to be solved. The interface of the library is inherited from the standard defined by OpenAI Gym, consisting of four main methods: gym.make(id), env.step(action), env.reset(), and env.render().

- Author: Edouard Leurent
- Contact: Edouard Leurent

<h1 style="text-align:center; color:red;">SIERRA Project-Team</h1>

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 Project-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
- 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 : Certifying the interoperability of RDF database systems using a continuous delivery workflow - 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 June 2019 Codalab exceeded 40,000 users, 1000 competitions (300 public), and had over 300 submissions per day. 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 by the Région Ile de France to organize its challenges in the next three years.

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 fith 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) and Université de Grenoble to use this platform as part of a curriculum of medical students. We created a special application called ChaGrade to grade homework using challenges. 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.

- 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: This year, Cartolabe was applied to the Grand Debat dataset (3M individual propositions from french Citizen, see https://cartolabe.fr/map/debat). The results were used to test both the scaling capabilities of Cartolabe and its flexibility to non-scientific and non-english corpuses. We also Added sub-map capabilities to display the result of a year/lab/word filtering as an online generated heatmap with only the filtered points to facilitate the exploration.

- Participants: Philippe Caillou, Jean-Daniel Fekete, Jonas Renault and Anne-Catherine Letournel
- Partners: LRI - Laboratoire de Recherche en Informatique - CNRS
- Contact: Philippe Caillou
- URL: http://www.cartolabe.fr/

5. New Software and Platforms

5.1. biips

Bayesian Inference with Interacting Particle Systems

KEYWORD: Bayesian estimation

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, François Caron, Pierre Del Moral and Pierrick Legrand
- 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

<p style="text-align:center; color:red;">**MATHRISK Project-Team**</p>

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. Premia

6.2.1. Development of the quantitative platform Premia in 2019

Premia 21 has been delivered to the Premia Consortium on March 21th 2019.
In this version, the following algorithms have been implemented:

6.2.1.1. Machine Learning, Risk Management, Risk model, Insurance

- Machine Learning for Quantitative Finance: Fast Derivative Pricing, Hedging and Fitting. J. De Spiegeleer, D. B. Madan, S. Reyners, W. Schoutens
  Quantitative Finance 2018
- Gaussian Process Regression for Pricing Variable Annuities with Stochastic Volatility and Interest Rate. L.Goudenege A.Molent A.Zanette 2019
- Machine Learning for Pricing American Options in High Dimension. L.Goudenege A.Molent A.Zanette 2019
- Neural networks for American options. L.Goudenege
- Sampling of probability measures in the convex order and approximation of Martingale Optimal Transport problems. A. Alfonsi, J. Corbetta, B. Jourdain
- Computing Credit Valuation Adjustment solving coupled PIDEs in the Bates model. L. Goudenege, A. Molent, A. Zanette
  Computational Management Science, to appear 2019

- Valuation of variable annuities with Guaranteed Minimum Withdrawal Benefit under stochastic interest rate. P.V.Shevchenko, X.Luo
  Insurance: Mathematics and Economics, Volume 76, 2017

6.2.1.2. Equity Derivatives

- An adjoint method for the exact calibration of Stochastic Local Volatility models. M.Wins, K.J.in 't Hout.
  Journal of Computational Science, Volume 24, 2018

- Discretization of class of diffusions nonlinear in the sense of McKean including the calibrated LVSV model. B. Jourdain, A. Zhou

- On an efficient multiple time-step Monte Carlo simulation of the SABR model. A. Leitao, L.A. Grzelak, C.W. Oosterlee
  Applied Mathematics and Computation, Vol. 293, 2017

- Robust Barrier Option Pricing by Frame Projection under Exponential Levy Dynamics. J.L. Kirkby
  Applied Mathematical Finance, Volume 24, Issue 4, 2017

- Ultra-Fast Pricing Barrier Options and CDSs. S.Levendorskii
  International Journal of Theoretical and Applied Finance, 20(5), 2017

- Efficient Binomial tree for the discretization of the CEV model. L.Caramellino, E.Lombardo.

- Pricing path-dependent Bermudan options using Wiener chaos expansion: an embarrassingly parallel approach. J.Lelong

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

SIMSMART Project-Team (section vide)

5. New Software and Platforms

5.1. diamss

KEYWORDS: High-performance calculation - Computation - Stochastic process

FUNCTIONAL DESCRIPTION: Numerical resolution of Keller-Segel equations and everal numerical tests.

- Participants: Denis Talay, Hector Olivero-Quinteros and Milica Tomasevic
- Contact: Denis Talay

5.2. ExitBM

FUNCTIONAL DESCRIPTION: The exitbm library provides methods to simulate random variables related to the first exit time and position of the Brownian motion from simple domains, namely intervals, squares and rectangles.

- Participants: Antoine Lejay and Madalina Deaconu
- Contact: Antoine Lejay
- URL: http://exitbm.gforge.inria.fr/

5.3. MOC

Models Of Chemostat

KEYWORD: Simulator

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

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

5.4. SDM

Stochastic Downsaling Method

FUNCTIONAL DESCRIPTION: The computation of the wind at small scale and the estimation of its uncertainties is of particular importance for applications such as wind energy resource estimation. To this aim, starting in 2005, we have developed a new method based on the combination of an existing Numerical Weather Prediction model providing a coarse prediction, and a Lagrangian Stochastic Model for turbulent flows. This Stochastic Downscaling Method (SDM) requires a specific modeling of the turbulence closure, and involves various simulation techniques whose combination is totally original (such as Poisson solvers, optimal transportation mass algorithm, original Euler scheme for confined Langevin stochastic processes, and stochastic particle methods).

- Participants: Antoine Rousseau, Antoine Rousseau, Claire Chauvin, Frederic Bernardin and Mireille Bossy
- Contact: Mireille Bossy

5.5. SDM-Log

- Participants: Antoine Rousseau, Claire Chauvin, Frederic Bernardin, Jacques Morice and Mireille Bossy
- Contact: Mireille Bossy

5.6. WindPoS-SDM-LAM

KEYWORDS: Numerical simulations - 3D - Fluid mechanics

FUNCTIONAL DESCRIPTION: Software platform for wind modeling.

- Authors: Antoine Rousseau, Cristian Paris Ibarra, Jacques Morice, Mireille Bossy and Sélim Kraria
- Contact: Mireille Bossy
- URL: https://windpos.inria.fr

5.7. WindPoS-ATM

KEYWORDS: 3D - Co-simulation - Fluid mechanics

- Authors: Philippe Drobinski, Antoine Rousseau, Mireille Bossy, Jacques Morice and Thomas Dubos
- Partners: Ecole Polytechnique - Laboratoire de Météorologie Dynamique
- Contact: Mireille Bossy
- URL: https://windpos.inria.fr/projects/windpos/

5.8. WindPoS-CIV

WinsPoS-CIV (Configuration Interface and Visualization)

- Authors: Sélim Kraria, Antoine Rousseau and Mireille Bossy
- Contact: Mireille Bossy

5.9. SBM

Skew Brownian Motion

KEYWORDS: Monte-Carlo methods - Skew Brownian Motion

FUNCTIONAL DESCRIPTION: SBM is a code allowing exact or approximated simulations of the Skew Brownian Motion. This code is used for the simulation, with a Monte-Carlo approach, of a 1D diffusion process with a discontinuous diffusion coefficient. Several benchmark tests are also implemented.

NEWS OF THE YEAR: - Refactoring and Cmake compilation - Automatic non regression tests on ci-inria.fr - Full documentation - Open source project on gitlab-inria

- Authors: Antoine Lejay and Géraldine Pichot
- Contact: Antoine Lejay
- Publication: Simulating diffusion processes in discontinuous media: Benchmark tests
- URL: https://gitlab.inria.fr/lejay/sbm