RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

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Section New Results

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STOCHASTIC APPROACHES

ACUMES Project-Team

7. New Results

7.1. Macroscopic traffic flow models on networks

Participants: Guillaume Costeseque, Paola Goatin, Bhargava Rama Chilukuri [Georgia Tech, USA], Maria Laura Delle Monache [U Rutgers - Camden], Aurélien Duret [IFSTTAR, France], Simone Göttlich [U Mannheim, Germany], Oliver Kolb [U Mannheim, Germany], Jorge A. Laval [Georgia Tech, USA], Benedetto Piccoli [U Rutgers - Camden], Armin Seyfried [Forschungszentrum Jülich, Germany], Antoine Tordeux [Forschungszentrum Jülich, Germany].

In collaboration with M.L. Delle Monache and B. Piccoli, and in the framework of the Associated Team ORESTE, we have introduced a new Riemann solver for traffic flow on networks. The Priority Riemann solver (PRS) provides a solution at junctions by taking into consideration priorities for the incoming roads and maximization of through flux. We prove existence of solutions for the solver for junctions with up to two incoming and two outgoing roads and show numerically the comparison with previous Riemann solvers. Additionally, we introduce a second version of the solver that considers the priorities as softer constraints and illustrate numerically the differences between the two solvers. See [24].

Still in collaboration with M.L. Delle Monache, we studied well-posedness of scalar conservation laws with moving flux constraints arising in the modeling of moving bottlenecks in traffic flow. In particular, we showed the Lipschitz continuous dependence of BV solutions with respect to the initial data and the constraint trajectory [23].

In collaboration with S. Göttlich and O. Kolb, we have investigated how second order traffic flow models, in our case the Aw-Rascle equations, can be used to reproduce empirical observations such as the capacity drop at merges and solve related optimal control problems. To this aim, we have proposed a model for on-ramp junctions and derive suitable coupling conditions. These are associated to the first order Godunov scheme to numerically study the well-known capacity drop effect, where the outflow of the system is significantly below the expected maximum. Control issues such as speed and ramp meter control have also been addressed in a first discretize-then optimize framework [25].

Together with J. A. Laval and B. R. Chilukuri, we have investigated the implications of source terms in the Hamilton-Jacobi formulation of macroscopic first order traffic flow models. Hamilton-Jacobi equations (without source terms) have been demonstrated to be very useful in traffic flow engineering since they provide explicit formula for initial and boundary-values problems. However, for sake of realism, additional source terms should be incorporated to account for continuous inflows or outflows on freeways for instance. We showed that explicit Lax-Hopf formula can still be obtained when the source term is exogenous, say the lateral inflow or outflow does not depend on the density on the main road. We also provide numerical methods based on Bellman's dynamic programming principle to deal with non-exogenous source terms in discrete time [7].

With A. Duret, we have designed a new traffic flow model for taking into account the multiclass and multilane features of real traffic. This model is based on a system of coupled Hamilton-Jacobi PDEs for an appropriate choice of framework that mixes spatial and Lagrangian coordinates. The coupling conditions emerge from the moving bottleneck theory that has been developed in the traffic flow literature several years ago but for which a real mathematical sound basis lacked. Very recently, there were some new results dealing with the existence of a solution under suitable assumptions [64]. However, these results were set for the hyperbolic conservation law in Eulerian coordinates and they are not straightforward to be extended to Hamilton-Jacobi equations in different coordinates. Despite that the well-posedness of the problem is still an open problem, a numerical method is developed by taking advantage of the classical representation formula available for HJ PDEs. This numerical scheme has been proved to provide good qualitative results [14].

In collaboration with A. Tordeux, M. Herty and A. Seyfried, we studied the derivation of convection-diffusion macroscopic traffic flow models from a first order microscopic follow-the-leader model that takes into account a non-trivial time delay. The derivation is based on a change of variables from Lagrangian to Eulerian coordinates and makes use of Taylor expansions with respect to the time delay. The macroscopic diffusion term is due to the microscopic reaction time parameter and allows to reproduce the scatter of empirical flow-density data. Different numerical methods are proposed for computing the numerical flux and the linear stability of the homogeneous solutions obtained for each method is investigated. Interestingly, we recover some stability results for infinite systems of delayed ODEs [27].

7.2. Initial-boundary value problems for non-local scalar conservation laws

Participants: Cristiana de Filippis, Paola Goatin.

As a first step in this direction, we have proved global well-posedness results for weak entropy solutions of bounded variation (BV) of scalar conservation laws with non-local flux on bounded domains in one space dimension, under suitable regularity assumptions on the flux function. In particular, existence is obtained by proving the convergence of an adapted Lax-Friedrichs algorithm. Lipschitz continuos dependence from initial and boundary data is derived applying Kružhkov 's doubling of variable technique [22].

7.3. High order schemes for non-local conservation laws

Participants: Paola Goatin, Christophe Chalons [UVST], Luis Miguel Villada Osorio [U Bio-Bio].

We have designed Discontinuous Galerkin (DG) schemes and Finite Volume WENO (FV-WENO) schemes to obtain high-order approximations of the solutions of a class of non-local conservation laws in one space dimension. The DG schemes give the best numerical results but their CFL condition is very restrictive. On the contrary, FV-WENO schemes can be used with larger time steps. The evaluation of the convolution terms necessitates the use of quadratic polynomials reconstructions in each cell in order to obtain the high-order accuracy with the FV-WENO approach. See [21].

7.4. Isogeometric analysis for hyperbolic systems

Participants: Régis Duvigneau, Asma Azaouzi [ENIT], Maher Moakher [ENIT].

The use of high-order numerical schemes is necessary to reduce numerical diffusion/dispersion in simulations, maintain a reasonable computational time for 3D problems, estimate accurately uncertainties or sensitivities, etc. Moreover, the capability to handle exactly CAD data in physical solvers is desirable to foster design optimization or multidisciplinary couplings.

Consequently, we develop high-order isogeometric schemes for the applications targeted by the team, in particular for convection-dominated problems. Specifically, we investigate a Discontinuous Galerkin method for compressible Euler equations, based on an isogeometric formulation: the partial differential equations governing the flow are solved on rational parametric elements, that preserve exactly the geometry of boundaries defined by Non-Uniform Rational B-Splines (NURBS), while the same rational approximation space is adopted for the solution. This topic is partially studied in A. Azaouzi's PhD work.

7.5. Sensitivity equation method for hyperbolic systems

Participants: Régis Duvigneau, Camilla Fiorini [UVST], Christophe Chalons [UVST].

While the sensitivity equation method is a common approach for parabolic systems, its use for hyperbolic ones is still tedious, because of the generation of discontinuities in the state solution, yielding Dirac distributions in the sensitivity solution.

To overcome this difficulty, we investigate a modified sensitivity equation, that includes an additional source term when the state solution exhibits discontinuities, to avoid the generation of delta-peaks in the sensitivity solution. We consider as example the one-dimensional barotropic Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach. This study is achieved in collaboration with C. Chalons from University of Versailles, in the context of C. FIorini's PhD work.

7.6. Characterization of model uncertainty for turbulent flows

Participants: Régis Duvigneau, Jérémie Labroquère [THALES], Emmanuel Guilmineau [CNRS-ECN], Marianna Braza [CNRS-IMFT], Mathieu Szubert [CNRS-IMFT].

The uncertainty related to turbulence modeling is still a bottleneck in realistic flows simulation. Therefore, some studies have been conducted to quantify this uncertainty for two problems in which turbulence plays a critical role. Firstly, the impact of the model choice has been estimated in the case of a massively detached flow over a 2D backward facing step including an oscillatory active control device, whose parameters are optimized [5]. Secondly, the influence of the transition point location has been investigated, in the case of the 3D flow around a bluff-body, using models ranging from RANS to DES models [9], in collaboration with M. Braza from Institut de Mécanique des Fluides de Toulouse, in the context of the M. Szubert's PhD work.

7.7. Optimization accounting for experimental and numerical uncertainties

Participants: Régis Duvigneau, Matthieu Sacher [Ecole Navale], Frédéric Hauville [Ecole Navale], Olivier Le Maître [CNRS-LIMSI], Alban Leroyer [CNRS-ECN], Patrick Queutey [CNRS-ECN].

Optimization of real-life applications requires to account for the uncertainties arising during the performance evaluation procedure, that could be either experimental or numerical. A Gaussian-Process based optimization algorithm has been proposed to efficiently determine the global optimum in presence of noise, whose amplitude can be user-defined or inferred from observations. The method has been applied to two very different problems related to performance optimization in sport.

The first case corresponds to the optimization of the shape of a racing kayak, in the framework of SOKA project, in preparation to 2016 Olympic Games. The performance is estimated by coupling Newton's law with incompressible Navier-Stokes equations to compute the kayak velocity from the effort of the athlete, considered as input. The proposed method has been used here to filter the noise arising from the numerical simulation [18], [11]. This work is conducted in collaboration with Ecole Centrale de Nantes and National Kayak Federation.

The second case corresponds to the optimization of a sail trimming, whose performance can be estimated either experimentally in a wind tunnel, or numerically by solving a fluid-structure interaction problem. In the former case, uncertainty has been estimated according to measurements accuracy, while in the latter case the numerical noise has be inferred from a set of observations collected during the optimization[12]. This work is part of M. Sacher's PhD at Ecole Navale.

7.8. Modeling activated/inhibited cell-sheet wound dynamics

Participants: Abderrahmane Habbal, Hélène Barelli [Univ. Nice Sophia Antipolis, CNRS, IPMC], Grégoire Malandain [Inria, EPI Morpheme], Boutheina Yahyaoui [PhD, LAMSIN, Univ. Tunis Al Manar], Mekki Ayadi [LAMSIN, Univ. Tunis Al Manar].

In a previous paper [91], we have shown that the well-known Fisher-KPP equations are able to model the natural wound closure of cell-sheets. This family of equations, with constant coefficients, exhibit progressive fronts with constant speed and we have proved by confronting to experiments that F-KPP is remarkabely able to predict the dynamics of experimental wounds. However, this is no more the case when the cell-sheet is either inhibited or activated exogeneously. In this case, we used a F-KKP equation with time-dependent coefficients, and proved again that with this modification we were able to capture the wound dynamics [13]. To take into account further biological features in the mathematical model, we implemented a coupling between the mechanical behavior of the cell tissue and the evolution of the density, using classical linear visco-elastic models from the literature. Our present effort is on assessing the ability of the mechano-biological coupled system to render some of the cell-sheet dynamics that are missing from the Fisher-KPP equation alone.

7.9. A Nash game for the coupled problem of conductivity identification and data completion

Participants: Abderrahmane Habbal, Rabeb Chamekh [PhD, LAMSIN, Univ. Tunis Al Manar], Moez Kallel [LAMSIN, Univ. Tunis Al Manar], Nejib Zemzemi [Inria Bordeaux, EPI CARMEN].

In this work, we are interested in solving the electrocardiography inverse problem which could be reduced to the data completion problem for the Poisson equation. The difficulty comes from the fact that the conductivity values of the torso organs like lungs, bones, liver,...etc, are not known and could be patient dependent. Our goal is to construct a methodology allowing to solve both data completion and conductivity optimization problems at the same time.

In [92], [101] a Nash game approach was developed to tackle the data completion problem. Our algorithm turned out to be efficient and robust with respect to noisy data. In a first attempt, presented in [17], we formulated the identification-completion problem as a Stackelberg game. Some numerical experiments were successful in this joint identification, but some were not. Which led us to develop new formulations, with direct impact on the technological modus operandi in the theoretical tomography process. In few words, the new formulations are based on the remark that not all the over-specified data are necessary to ensure the existence and uniqueness for the Cauchy problem, since by Holmgren theorem, only a piece of these data (over a subset of the boundary with non zero superficial measure) is necessary and sufficient. Presently, we are investigating the ability of these new formulations to ensure identifiability of the conductivity coefficients, for Poisson and linear elasticity equations.

7.10. Bayesian Optimization approaches to find Nash equilibria

Participants: Mickael Binois [Univ. of Chicago], Victor Picheny [INRA, Toulouse], Abderrahmane Habbal.

Our aim here is to show that the Bayesian Optimization -BO- apparatus can be applied to the search of game equilibria, and in particular the classical Nash equilibrium (NE), known to be very costly the compute, notably when involved in the framework of large scale scientific computing areas.

BO relies on Gaussian processes, which are used as emulators (or surrogates) of the black-box model outputs based on a small set of model evaluations. Posterior distributions provided by the Gaussian process are used to design *acquisition functions* that guide sequential search strategies that balance between exploration and exploitation.

We have proposed in [26] a novel approach to solve Nash games with drastically limited budgets of evaluations based on GP regression, taking the form of a Bayesian optimization algorithm. Experiments on challenging benchmark problems demonstrate the potential of this approach compared to classical, derivative-based algorithms.

On the test problems, two acquisition functions performed similarly well. The first one, Stepwise Uncertainty Reduction -SUR- has recently emerged in the machine learning community. We introduced a new one, the Probability of Equilibrium P_E, which has the benefit of not relying on conditional simulation paths, which makes it simpler to implement and less computationally intensive in most cases. Still, the SUR approach has several decisive advantages; in particular, it does not actually require the new observations to belong to the grid (sampling of the , such that it could be optimized continuously. Moreover, it lays the groundwork for many extensions that may be pursued in future work.

First, SUR strategies are well-suited to allow selecting batches of points instead of only one, a key feature in distributed computer experiments. Second, other games and equilibria may be considered: the versatility of the SUR approach may allow its transposition to other frameworks, such as mixed-strategies or Bayesian games. In particular, our framework transposes directly to the case of noisy evaluations, as it can be directly modeled by the GPs without affecting the acquisition functions.

7.11. Crowd motion modeled by Fokker-Planck constrained Nash games

Participants: Alfio Borzí [Univ. Würzburg], Paola Goatin, Abderrahmane Habbal, Souvik Roy [Indian Statistical Institute, Kolkata].

Fokker-Planck-Kolmogorov (FPK) equations are PDEs which govern the dynamics of the probability density function (PDF) of continuous-time stochastic processes (e.g. Ito processes). In [36] a FPK-constrained control framework, where the drift was considered as control variable is developed and applied to crowd motion.

We consider in [42] the extension of the latter framework to the case where two crowds (or pedestrian teams) are competing through a Nash game. The players strategies are the drifts, which yield two uncoupled FPK equations for the corresponding PDFs. The interaction is done through cost functions : each player would prefer to avoid overcrowding (w.r.t. the other one, hence the coupling) additionally to have her own preferred trajectory and obstacle avoidance. In this particular setting, we prove the existence and uniqueness of the Nash equilibrium (NE). The NE is computed by means of a fixed point algorithm and adjoint-state method is used to compute the pseudo-gradients. We finally present some numerical experiments to illustrate which dynamics may arise from such equilibria.

7.12. Concurrent Aerodynamic Optimization of Rotor Blades Using a Nash Game Method

Participants: Enric Roca León [ONERA DAAP Meudon, doctoral student], Arnaud Le Pape [ONERA DAAP Meudon, research engineer], Michel Costes [ONERA DAAP Meudon, research engineer], Jean-Antoine Désidéri, David Alfano [Airbus Helicopters].

A multiobjective strategy adapted to the aerodynamic concurrent optimization of helicopter rotor blades is developed. The present strategy is based on Nash games from game theory, where the objective functions are minimized by virtual players involved in a noncooperative concurrent game. A method is presented to split the design vector into two subspaces, defined to be the strategies of the players in charge of the minimization of the primary and the secondary objective functions, respectively. This split of territory allows the optimization of the secondary function while causing the least possible degradation of the first one. This methodology is applied to the model rotor ERATO, seeking to maximize the figure of merit in hover while minimizing the required rotor power in forward flight, assuming frozen structural properties. An initial constrained optimization in hover is conducted using a previously developed adjoint-based technique using the three-dimensional Navier–Stokes solver elsA along with the gradient-based CONMIN algorithm. The chord, twist, and sweep distributions of the baseline blade are parameterized using Bézier and cubic splines for a total of 16 design variables. The obtained optimized rotor is then used as a starting point to launch constrained and unconstrained Nash games. The comprehensive rotor code Eurocopter's Helicopter Overall Simulation Tool (HOST) is used to evaluate forward flight performance, and a surrogate model is built to obtain the hover performance at low computational cost. Twist and sweep distribution laws are optimized independently at first, and then a final joint optimization involving twist, sweep, and chord is performed. The results demonstrate the potential of this technique to obtain helicopter rotor designs realizing interesting trade-offs between strongly antagonistic objectives [8].

7.13. Parametric optimization of pulsating jets in unsteady flow by Multiple-Gradient Descent Algorithm (MGDA)

Participants: Jean-Antoine Désidéri, Régis Duvigneau.

Two numerical methodologies are combined to optimize six design characteristics of a system of pulsating jets acting on a laminar boundary layer governed by the compressible Navier-Stokes equations in a time-periodic regime. The flow is simulated by second-order in time and space finite-volumes, and the simulation provides the drag as a function of time. Simultaneously, the sensitivity equations, obtained by differentiating the governing equations w.r.t. the six parameters are also marched in time, and this provides the six-component parametric gradient of drag. When the periodic regime is reached numerically, one thus disposes of an objective-function, drag, to be minimized, and its parametric gradient, at all times of a period. Second, the parametric optimization is conducted as a multi-point problem by the Multiple-Gradient Descent Algorithm (MGDA) which permits to reduce the objective-function at all times simultaneously, and not simply in the sense of a weighted average [19].

7.14. Stochastic Multiple Gradient Descent Algorithm

Participants: Jean-Antoine Désidéri, Quentin Mercier [ONERA DADS Châtillon, doctoral student], Fabrice Poirion [ONERA DADS Châtillon, research engineer].

We have proposed a new method for multiobjective optimization problems in which the objective functions are expressed as expectations of random functions. This method is based on an extension of the classical stochastic gradient algorithm and a deterministic multiobjective algorithm, the Multiple-Gradient Descent Algorithm (MGDA). In MGDA a descent direction common to all specified objective functions is identified through a result of convex geometry. The use of this common descent vector and the Pareto stationarity definition into the stochastic gradient algorithm makes the algorithm able to solve multiobjective problems. The mean square and almost sure convergence of this new algorithm are proven considering the classical stochastic gradient algorithm hypothesis. The algorithm efficiency is illustrated on two academic examples and its performance is compared to the deterministic MGDA algorithm coupled with a Monte-Carlo expectation estimator. A third example is treated, considering the optimization of a sandwich material under constitutive material uncertainties.

7.15. Finite-volume goal-oriented mesh adaptation for aerodynamics using functional derivative with respect to nodal coordinates

Participants: Giovanni Todarello [ONERA DMFN Châtillon, intern], Floris Vonck [ONERA DMFN Châtillon, intern], Sébastien Bourasseau [ONERA, doctoral student], Jacques Peter [ONERA DMFN Châtillon, research engineer], Jean-Antoine Désidéri.

A new goal-oriented mesh adaptation method for finite volume/finite difference schemes is extended from the structured mesh framework to a more suitable setting for adaptation of unstructured meshes. The method is based on the total derivative of the goal with respect to volume mesh nodes that is computable after the solution of the goal discrete adjoint equation. The asymptotic behaviour of this derivative is assessed on regularly refined unstructured meshes. A local refinement criterion is derived from the requirement of limiting the first order change in the goal that an admissible node displacement may cause. Mesh adaptations are then carried out for classical test cases of 2D Euler flows. Efficiency and local density of the adapted meshes are presented. They are compared with those obtained with a more classical mesh adaptation method in the framework of finite volume/finite difference schemes [46]. Results are very close although the present method only makes usage of the current grid [10].

7.16. Quasi-Riemannian approach to constrained optimization

Participants: Didier Bailly [Research Engineer, ONERA Department of Applied Aerodynamics, Meudon], Jean-Antoine Désidéri.

In differentiable optimization, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method is one of the most efficient methods for unconstrained problems. Besides function values, it only requires the specification of the gradient. An approximate Hessian is calculated by successive approximations as part of the iteration, using rank-1 correction matrices. As a result, the iteration has superlinear convergence : when minimizing a quadratic function in n variables, if the one-dimensional minimizations in the calculated directions of search are done exactly, the Hessian matrix approximation is exact after n iterations, and from this, the iteration identifies to Newton's iteration, and produces the exact local optimum in only one additional iteration ($n+1$ in total).

However the BFGS method does extend to constrained problems very simply. Following Gabay [82] and other authors, Chunhong Qi *et al* [120] have proposed a "Riemannian" variant, RBFGS that indeed incorporates equality constraints in the formulation and actually demonstrates superior convergence rates for problems with a large number of variables. However these Riemannian formulations are non trivial to implement since they require procedures implementing non-trivial differential-geometry operators ('retraction' and 'metric transport') to be developed. In their paper, they assume a formal expression of the constraint to be known. But, in PDE-constrained optimization, many constraints are functional, and it is not clear how can the metric transport operator in particular can be defined.

We are investigating how can a quasi-Riemannian method can be defined based on the sole definition of evaluation procedures for the gradients. By condensing all the equality constraints in one, a purely-explicit approximate retraction operator has been defined that yields a point whose distance to the contraint surface is fourth-order at least. The associated transport operator is currently being examined formally. These techniques will be experimented in the context of constrained optimum-shape design in aerodynamics [20]

7.17. Multifidelity surrogate modeling based on Radial Basis Functions

Participants: Jean-Antoine Désidéri, Cédric Durantin [CEA LETI Grenoble, doctoral student], Alain Glière [CEA LETI Grenoble, research engineer], Justin Rouxel [CEA LETI Grenoble, doctoral student].

Multiple models of a physical phenomenon are sometimes available with different levels of approximation. The high fidelity model is more computation-ally demanding than the coarse approximation. In this context, including information from the lower fidelity model to build a surrogate model is desirable. Here, the study focuses on the design of a miniaturized photoacoustic gas sensor which involves two numerical mod- els. First, a multifidelity metamodeling method based on Radial Basis Function, the co-RBF, is proposed. This surrogate model is compared with the classical co-kriging method on two analytical benchmarks and on the photoacoustic gas sensor. Then an extension to the multifidelity framework of an already existing RBF- based optimization algorithm is applied to optimize the sensor efficiency. The co-RBF method brings promising results on a problem in larger dimension and can be considered as an alternative to co-kriging for multifidelity metamodeling.

CAGIRE Project-Team

7. New Results

7.1. Heat transfer for effusion flows

The conjugate heat-transfer problem of a flow around a multi- perforated plate under realistic conditions has been addressed by the coupling of the LES-AVBP solver for the flow and the AVTP for solving the heat equation in the solid. A description of the topology of the heat exchange has been realized for the aspiration and injection sides of the walls as well as in the inner side of the holes. This work highlights the potential of such a fluid-solid coupling strategy in the description of the heat exchange distribution for combustor liners. Different analytical expressions have been assessed for each category of exchange surface.[15]

7.2. All-Mach numerical fluxes

This study was split into three self-consistent parts. In the first one, the low Mach number problem through a linear analysis of a perturbed linear wave equation was defined and analyzed. Then, we show how to modify Godunov type schemes applied to the linear wave equation to make this scheme accurate at any Mach number. This allows to define an all Mach correction and to propose a linear all Mach Godunov scheme for the linear wave equation. In the second one, we apply the all Mach correction proposed previously to the case of the non-linear barotropic Euler system when the Godunov type scheme is a Roe scheme. A linear stability result is proposed and a formal asymptotic analysis justifies the construction in this non-linear case by showing how this construction is related with the linear analysis. At last, we apply the all Mach correction to the case of the full Euler compressible system. Numerous numerical results justify the theoretical results and show that the obtained all Mach Godunov type schemes are both accurate and stable for all Mach numbers. We also underline that the proposed approach can be applied to other schemes and allows to justify other existing all Mach schemes.

7.3. Extension and validation of the EB-RSM model

The EB-RSM RANS turbulence model, an innovative model based on second moment closure, has been developed for almost 15 years and is now gradually deployed in the industrial practise. It is already implemented in several industrial codes (Code_Saturne, StarCCM+, EZNSS), as well as the open-source code OpenFOAM. In collaboration with industrial partners, the model is now being confronted to more and more complex industrial configurations: Wall-cooling using impinging jets; Measurement/control of head losses in pipes or injectors via local restrictions of the section (diaphragms); Turbine blade cooling by pin matrices; Control of boundary layer separation by local blowing to exploit the Coanda effect; Wing-tip vortices around airfoils representative of the spoilers of Formula One racing cars; Open-water propeller. All these results confirm the interest of the model compared to well-established models, and its numerical robustness.

7.4. Creation of a database of a direct numerical simulation of a jet in cross flow with and without gyration and with non isothermal flows

This year, we performed the direct numerical simulation of a jet in cross flow without gyration and with a 90° skidding with respect to the cross flow, and with a cross flow 800 Kelvin hotter than the jet. The Sutherland law was implemented for accounting for viscous effects in the non isothermal case and was validated. Then direct numerical simulations have been performed, by using synthetic eddy methods for inlet boundary conditions. Third order discretization was used. A limiter on the density was also used for damping oscillations in strong shear layers, which in this case include both large density and velocity gradients.

The database contains the mean flow at all points, the Reynolds tensor at the degrees of freedom, and the time dependent data at some probes.

CARDAMOM Project-Team

6. New Results

6.1. High order discretizations on unstructured meshes

- Participants: Héloise Beaugendre, Cécile Dobrzynski, Léo Nouveau, Mario Ricchiuto, Quentin Viville
- Corresponding member: Héloise Beaugendre

Our work on high order unstructured discretizations this year has pursued three main avenues:

- We have extended the team's previous work on the consistent residual based approximation of viscous flow equations to the framework of Immersed Boundary Methods (IBM). This is an increasingly popular approach in Computational Fluid Dynamics as it simplifies the mesh generation problem. In our work, we consider a technique based on the addition of a penalty term to the Navier-Stokes equations to account for the wall boundary conditions. To adapt the residual distribution method method to the IBM, we developed a new formulation based on a Strang splitting appproach in time. This approach, couples in a fully consistent manner an implicit asymptoticly exact integration procedure of the penalization ODE, with the explicit residual distribution discretization for the Navier-Stokes equations, based on the method proposed in [122]. The ODE integrator provides an operator which is exact up to orders η^2, with η the penalty parameter assuming values of the order of 10^{-10}. To preserve the accuracy of the spatial discretization in the Navier-Stokes step, we have introduced, in vicinity of the penalised region, a modification of the solution gradient reconstruction required for the evaluation of the viscous fluxes. We have shown formally and numerically that the approach proposed is second order accurate for smooth solutions, and shown its potential when combined with unstructured mesh adaptation strategies w.r.t. the (implicitly described) solid walls [16]. This approach has been combined with $r-$adaptation techniques to account for moving bodies and validated on simulations involving flapping wings, and computations of ices block trajectories in the framework of the STORM project [56], [46];
- Another research axis consists in proposing a novel approach that allows to use p-adaptation with continuous finite elements. Under certain conditions, primarily the use of a residual distribution scheme, it is possible to avoid the continuity constraint imposed to the approximate solution, while still retaining the advantages of a method using continuous finite elements. The theoretical material, the complete numerical method and practical results show as a proof of concept that p-adaptation is possible with continuous finite elements. This year, we extended the p-adaptation method to Navier-Stokes equations and coupled it with immersed boundary method.
- We have studied the high order approximation of problems with dispersion and suggested a route allowing to construct high order methods (up to order 4) allowing to obtain the same accuracy for the solution, and for its first and second order derivatives. Initial validation for the approach proposed has been shown for the time dependent KdV equations [14], [49].

6.2. High order mesh generation and mesh adaptation

- Participants: Luca Arpaia , Cécile Dobrzynski, Ghina El Jannoun, Léo Nouveau, Mario Ricchiuto
- Corresponding member: Cécile Dobrzynski

This year several new algorithmic improvements have been obtained which will allow to enhance our meshing tools:

- We have enhanced our work on r-adaptation techniques for time dependent equations. These techniques are based on mesh deformations obtained by solving continuous differential equations for the local displacements. These equations are controlled by an error monitor. Several improvements have been made. We have studied in depth the formulation of the coupling of the mesh movement with the flow solver. We have found that for both finite volume and residual distribution methods, a coupling of mesh and solution evolution (by means of an ALE method) provides accuracy enhancements, and is to be preferred to a simpler adapt-project-evolve approach. The method has been fully tested in two space dimensions and preliminary results have been performed in three dimensions. We have applied this technic to immersed boundary methods to compressible simulations. For problems with source terms, and in particular problems admitting some important physical invariants as the shallow water equations, we have solved the conflict between the conservation of either mass or the invariant, allowing for the conservation of both quantities up to machine accuracy. In parallel we have proposed a modified formulation of an elasticity equation allowing to reduce the nonlinearity of the mesh PDE to the force imposed in the right hand side. Initial validation has been shown in [56] and in the PhD of L. Nouveau ;

6.3. Uncertainty Quantification and robust design optimization

- Participants: Andrea Cortesi , Pietro Marco Congedo, Nassim Razaaly, Sanson Francois
- Corresponding member: Pietro Marco Congedo

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

Concerning sensitivity analysis, we illustrate how third and fourth-order moments, i.e. skewness and kurtosis, respectively, can be decomposed mimicking the ANOVA approach. It is also shown how this decomposition is correlated to a Polynomial Chaos (PC) expansion leading to a simple strategy to compute each term. New sensitivity indices, based on the contribution to the skewness and kurtosis, are proposed. The outcome of the proposed analysis is depicted by considering several test functions. Moreover, the ranking of the sensitivity indices is shown to vary according to their statistics order. Furthermore, the problem of formulating a truncated polynomial representation of the original function is treated. Both the reduction of the number of dimensions and the reduction of the order of interaction between parameters are considered. In both cases, the impact on the reduction is assessed in terms of statistics, namely the probability density function. Feasibility of the proposed analysis in a real-case is then demonstrated by presenting the sensitivity analysis of the performances of a turbine cascade in an Organic Rankine Cycles (ORCs), in the presence of complex thermodynamic models and multiple sources of uncertainty.

Moreover, we have developed a new framework for performing robust design optimization. a strategy is developed to deal with the error affecting the objective functions in uncertainty-based optimization. We refer to the problems where the objective functions are the statistics of a quantity of interest computed by an uncertainty quantification technique that propagates some uncertainties of the input variables through the system under consideration. In real problems, the statistics are computed by a numerical method and therefore they are affected by a certain level of error, depending on the chosen accuracy. The errors on the objective function can be interpreted with the abstraction of a bounding box around the nominal estimation in the objective functions space. In addition, in some cases the uncertainty quantification methods providing the objective functions also supply the possibility of adaptive refinement to reduce the error bounding box. The novel method relies on the exchange of information between the outer loop based on the optimization algorithm and the inner uncertainty quantification loop. In particular, in the inner uncertainty quantification loop, a control is performed to decide whether a refinement of the bounding box for the current design is appropriate or not. In single-objective problems, the current bounding box is compared to the current optimal design. In multi-objective problems, the decision is based on the comparison of the error bounding box of the current design and the current Pareto front. With this strategy, fewer computations are made for clearly dominated solutions and an accurate estimate of the objective function is provided for the interesting, non-dominated solutions. The results presented in this work prove that the proposed method improves the efficiency of the global loop, while preserving the accuracy of the final Pareto front.

Concerning semi-intrusive methods, a novel multiresolution framework, namely the Truncate and Encode (TE) approach is generalized and extended for taking into account uncertainty in partial differential equations (PDEs). Innovative ingredients are given by an algorithm permitting to recover the multiresolution representation without requir- ing the fully resolved solution, the possibility to treat a whatever form of pdf and the use of high-order (even non-linear, i.e. data-dependent) reconstruction in the stochastic space. Moreover, the spatial-TE method is introduced, which is a weakly intrusive scheme for uncertainty quantification (UQ), that couples the physical and stochastic spaces by minimizing the computational cost for PDEs. The proposed scheme is particularly attractive when treating moving discontinuities (such as shock waves in compressible flows), even if they appear during the simulations as it is common in unsteady aerodynamics applications. The proposed method is very flexible since it can easily coupled with different deterministic schemes, even with high-resolution features. Flexibility and performances of the present method are demonstrated on various numerical test cases (algebraic functions and ordinary differential equations), including partial differential equations, both linear and non-linear, in presence of randomness.

We applied a part of this method to a problem associated to the atmospheric reentry. In fact, an accurate determination of the catalytic property of thermal protection materials is crucial to design reusable atmospheric entry vehicles. This property is determined by combining experimental measurements and simulations of the reactive boundary layer near the material surface. The inductively-driven Plasmatron facility at the von Karman Institute for Fluid Dynamics provides a test environment to analyze gas-surface interactions under effective hypersonic conditions. In this study, we develop an uncertainty quantification methodology to rebuild values of the gas enthalpy and material catalytic property from Plasmatron experiments. A non-intrusive spectral projection method is coupled with an in-house boundary-layer solver, to propagate uncertainties and provide error bars on the rebuilt gas enthalpy and material catalytic property, as well as to determine which uncertainties have the largest contribution to the outputs of the experiments. We show that the uncertainties computed with the methodology developed are significantly reduced compared to those determined using a more conservative engineering approach adopted in the analysis of previous experimental campaigns.

6.4. Modelling of free surface flows

- Participants: Luca Arpaia , Stevan Bellec , Mathieu Collin , Sebastien De Brye , Andrea Filippini , Maria Kazolea, Luc Mieussens, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

We have introduced a new systematic method to obtain discrete numerical models for incompressible free-surface flows. our approach allows to recover discrete asymptotic equations from a semi-discretized form

(keeping the vertical z variable and time continuous) of the incompressible Euler equations with free surface. In particular, starting from a (continuous) Galerkin finite element discretization in the horizontal direction, we perform an asymptotic analysis of the resulting semi-discrete system. This has allowed to obtain new discrete equivalents of the Peregrine equations [5], as well as enhanced variants in the spirit of [115]. This has been done in the PhD of S. Bellec. We have demonstrated that the resulting discrete equations present dispersion characteristics much improved w.r.t. those obtained by directly discretizing the asymptotic Boussinesq equations with continuous finite elements. This has been confirmed by numerical experiments on long wave propagation benchmarks. Concerning more classical continuous Boussinesq models, additional work has been done to characterize some of their exact solutions. This has provided some improved solutions to benchmark our codes, as well as some additional knownledge on these models [4].
This year we extended our work on fully non-linear weakly dispersive wave models in two dimensional horizontal coordinates. The proposed framework in [11], to approximate the so-called Green-Naghdi equations is followed. The method proposed, while remaining unsplit in time, is based on a separation of the elliptic and hyperbolic components of the equations. This separation is designed to recover the standard shallow water equations in the hyperbolic step, so that the method can be written as an *algebraic* correction to an existing shallow water code. More precisely, we re-write the standard form of the equations by splitting the original system in its elliptic and hyperbolic parts, through the definition of a new variable, accounting for the dispersive effects and having the role of a non-hydrostatic pressure gradient in the shallow water equations. We consider a two-step solution procedure. In the first step we compute a source term by inverting the elliptic coercive operator associated to the dispersive effects; then in a hyperbolic step we evolve the flow variables by using the non-linear shallow water equations, with all nonhydrostatic effects accounted by the source computed in the elliptic phase. The advantages of this procedure are firstly that the GN equations are used for propagation and shoaling, while locally reverting to the non-linear shallow water equations to model energy dissipation in breaking regions. Secondly and from the numerical point of view, this strategy allows each step to be solved with an appropriate numerical method on arbitrary unstructured meshes. We propose a hybrid finite element (FE) finite volume (FV) scheme, where the elliptic part of the system is discretized by means of the continuous Galerkin FE method and the hyperbolic part is discretized using a third-order node-centered finite volume (FV) technique. This work was a part of Andrea Filippini's PhD and a research paper is under preparation.
We also continue our study on wave breaking techniques on unstructured meshes [55]. In particular, we evaluate the coupling of both a weakly and a fully non-linear Boussinesq system with a turbulence model. We reformulate an evolution model for the turbulent kinetic energy, initially proposed by Nwogu [115], and evaluate its capabilities to provide sufficient dissipation in breaking regions. We also compare this dissipation to the one introduced by the numerical discretization. A research paper on the topic, is under preparation. Further more we studied and tested the application and validation of TUCWave code on the transformation breaking and run-up of irregular waves. Its is the first time that an unstructured high-resolution FV numerical solver for the 2D extended BT equations of Nwogu is tested on the generation and propagation of irregular waves. A research paper is under preparation.

The tools developed have been also used intensively in funded research programs. Within the TANDEM project, several benchmarks relevant to tsunami modelling have been performed and several common publications with the project partners are submitted and/or in preparation [54], [45]. We also our code SLOWS, to study the conditions for tidal bore formation in convergent alluvial estuaries [7]. A new set of dimensionless parameters has been introduced to describe the problem, and the code SLOWS has been used to explore the space of these parameters allowing to determine a critical curve allowing to characterize an estuary as "bore forming" or not. Surprising physical behaviours, in terms of dissipation and nonlinearity of the tides, have been highlighted.

Finally, in collaboration with F. Veron (University of Delaware at Newark, USA), L. Mieussens has developed a model to describe the effect of rain falling on water waves [20]. This model is based on a kinetic description of rain droplets that is used to compute the induced pression on a water wave. This allows to estimate the dissipation (or amplification) of the wave due to rainy conditions.

6.5. Wave energy conversion hydrodynamics

- Participants: Umberto Bosi, Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

We have developed a prototype spectral element solver four a coupled set of differential equations modelling wave propagation (so-called outer domain), and the submerged flow under a floating body (inner domain). Both systems of equations are depth-averaged (Boussinesq type) systems involving some dispersive terms. They are further coupled to a force balance providing a (system of) ODE(s) for the floater. This model constitutes an intermediate fidelity approximation for the hydrodynamics of a wave energy converter. Differently from all industrial state of the art, it is a (fully) nonlinear model. However, its cost is extremely low when compared to full three-dimensional CFD analyses, due to the dimensional reduction brought from the depth averaged modelling. Last year we have shown the potential of this approach to predict the hydrodynamics of a floater in a simplified case [90], [91] (journal version to appear on *J. Ocean Eng. and Marine Energy*). This year we have further studied the issue of the coupling between domains with different PDE models (as in our case the inner and outer domains), and suggested an approach (based on a first order reformulation) allowing to coupled domains with different equations and with or without dispersive effects on either side. This work is done in the framework of the MIDWEST project funded by the EU OCEANEranet call.

DEFI Project-Team

7. New Results

7.1. Methods for inverse problems

7.1.1. Identifying defects in an unknown background using differential measurements

L. Audibert and H. Haddar

In the framework of the PhD thesis of Lorenzo Audibert we studied non destructive testing of concrete using ultrasonic waves, and more generallly imaging in complex heterogeneous media. We assume that measurements are multistatic, which means that we record the scattered field on different points by using several sources. For this type of data we wish to build methods that are able to image the obstacle that created the scattered field. We use qualitative methods in this work, which only provide the support of the object independently from its physical property. The first part of this thesis consists of a theoretical analysis of the Linear Sampling Method. Such analysis is done in the framework of regularization theory, and our main contribution is to provide and analyze a regularization term that ensures good theoretical properties. Among those properties we were able to demonstrate that when the regularization parameter goes to zero, we actually construct a sequence of functions that strongly converges to the solution of the interior transmission problem. This behavior gives a central place to the interior transmission problem as it allows describing the asymptotic solution of our regularized problem. Using this characterization of our solution, we are able to give the optimal reconstruction we can get from our method. More importantly this description of the solution allows us to compare the solution coming from two different datasets. Based on the result of this comparison, we manage to produce an image of the connected component that contains the defect which appears between two measurement campaigns and this regardless of the medium. This method is well suited for the characteristics of the microstructure of concrete as shown on several numerical examples with realistic concrete-like microstructure. Finally, we extend our theoretical results to the case of limited aperture, anisotropic medium and elastic waves, which correspond to the real physics of the ultrasounds

7.1.2. Generalized linear sampling method for elastic-wave sensing of heterogeneous fractures

B. Guzina, H. Haddar and F. Pourahmadian

A theoretical foundation is developed for active seismic reconstruction of fractures endowed with spatially-varying interfacial condition (e.g. partially-closed fractures, hydraulic fractures). The proposed indicator functional carries a superior localization property with no significant sensitivity to the fracture's contact condition, measurement errors, and illumination frequency. This is accomplished through the paradigm of the F-factorization technique and the recently developed Generalized Linear Sampling Method (GLSM) applied to elastodynamics. The direct scattering problem is formulated in the frequency domain where the fracture surface is illuminated by a set of incident plane waves, while monitoring the induced scattered field in the form of (elastic) far-field patterns. The analysis of the well-posedness of the forward problem leads to an admissibility condition on the fracture's (linearized) contact parameters. This in turn contributes toward establishing the applicability of the F-factorization method, and consequently aids the formulation of a convex GLSM cost functional whose minimizer can be computed without iterations. Such minimizer is then used to construct a robust fracture indicator function, whose performance is illustrated through a set of numerical experiments. For completeness, the results of the GLSM reconstruction are compared to those obtained by the classical linear sampling method.

7.1.3. Invisibility in scattering theory

L. Chesnel, A.-S. Bonnet-Ben Dhia and S.A. Nazarov

We are interested in a time harmonic acoustic problem in a waveguide with locally perturbed sound hard walls. We consider a setting where an observer generates incident plane waves at $-\infty$ and probes the resulting scattered field at $-\infty$ and $+\infty$. Practically, this is equivalent to measure the reflection and transmission coefficients respectively denoted R and T. In a recent work, a technique has been proposed to construct waveguides with smooth walls such that $R = 0$ and $|T| = 1$ (non reflection). However the approach fails to ensure $T = 1$ (perfect transmission without phase shift). First we establish a result explaining this observation. More precisely, we prove that for wavenumbers smaller than a given bound $k_{☆}$ depending on the geometry, we cannot have $T = 1$ so that the observer can detect the presence of the defect if he/she is able to measure the phase at $+\infty$. In particular, if the perturbation is smooth and small (in amplitude and in width), $k_{☆}$ is very close to the threshold wavenumber. Then, in a second step, we change the point of view and, for a given wavenumber, working with singular perturbations of the domain, we show how to obtain $T = 1$. In this case, the scattered field is exponentially decaying both at $-\infty$ and $+\infty$. We implement numerically the method to provide examples of such undetectable defects.

7.1.4. Nanoparticles volume determination from SAXS measurements

H. Haddar and Z. Jiang

The aim of this work is to develop a fully automatic method for the reconstruction of the volume distribution of polydisperse non-interacting nanoparticles with identical shapes from Small Angle X-ray Scattering measurements. In the case of diluted systems we proposed a method that solves a maximum likelihood problem with a positivity constraint on the solution by means of an Expectation Maximization iterative scheme coupled with a robust stopping criterion. We prove that the stopping rule provides a regularization method according to an innovative notion of regularization specifically defined for inverse problems with Poisson data. Such a regularization, together with the positivity constraint results in high fidelity quantitative reconstructions of particle volume distributions making the method particularly effective in real applications. We tested the performance of the method on synthetic data in the case of uni- and bi-modal particle volume distributions. We extended the method to the case of dense solutions where the inverse problem becomes non linear. A specific fix-point algorithm has been proposed and convergence has been tested against synthetic data. The developement of this research topic is ongoing under the framework of Saxsize.

7.1.5. Identifying defects in unknown periodic layers

H. Haddar and T.P. Nguyen

We investigate the inverse problem where one is interested in reconstructing the support of a perturbation in a periodic media from measurements of scattered waves. We are concerned with the design of a sampling method that would reconstruct the support of inhomogeneities without reconstructing the index of refraction. The development of sampling methods has gained a large interest in recent years and many methods have been introduced in the literature to deal with a variety of problems and we refer to [1] for an account of recent developments of these methods. Up to our knowledge, the sampling methods for locally perturbed infinite periodic layers has not been treated in the literature. Even thought this problem is the one that motivates our study, we considered a slightly different problem that will be referred to as the ML-periodic problem: it corresponds with a locally perturbed infinite periodic layer with period L that has been reduced to a domain of size ML (with M a sufficiently large parameter) with periodic boundary conditions. This is mainly for technical reasons since our analysis for the newly introduced differential imaging functional heavily rely on the discrete Floquet-Bloch transform.

The main contribution of our work is the design of a new sampling method that enable the imaging of the defect location without reconstructing the L periodic background. This method is in the spirit of the Differential LSM introduced above for the imaging of defects in complex backgrounds using differential measurements. However, in the present case we propose a method that does not require the measurement operator for the background media. We exploit the L periodicity of the background and the Floquet-Bloch transform to design a differential criterion between different periods. This criterion is based on the study of sampling methods for the ML-periodic media where a single Floquet-Bloch mode is used. This study constitutes the main theoretical ingredient for our method. The sampling operator for a single Floquet-Bloch mode somehow plays the role of the measurement operator for the background media. Indeed the main interest for this new sampling method is that it is capable of identifying the defect even thought classical sampling methods fail in obtaining high fidelity reconstructions of the (complex) background media.

7.1.6. Identification of small objects with near-field data in quasi-backscattering configurations

H. Haddar and M. Lakhal

We present a new sampling method for detecting targets (small inclusions or defects) immersed in a homogeneous medium in three-dimensional space, from measurements of acoustic scattered fields created by point source incident waves. We consider the harmonic regime and a data setting that corresponds with quasi-backscattering configuration: the data is collected by a set a receivers that are distributed on a segment centered at the source position and the device is swept along a path orthogonal to the receiver line. We assume that the aperture of the receivers is small compared with the distance to the targets. Considering the asymptotic form of the scattered field as the size of the targets goes to zero and the small aperture approximation, one is able to derive a special expression for the scattered field. In this expression a separation of the dependence of scattered field on the source location and the distance source-target is performed. This allows us to propose a sampling procedure that characterizes the targets location in terms of the range of a near-field operator constructed from available data. Our procedure is similar to the one proposed by Haddar-Rezac for far-field configurations. The reconstruction algorithm is based on the MUSIC (Multiple SIgnal Classification) algorithm.

7.1.7. Nondestructive testing of the delaminated interface between two materials

F. Cakoni, I. De Teresa, H. Haddar and P. Monk

We consider the problem of detecting if two materials that should be in contact have separated or delaminated. The goal is to find an acoustic technique to detect the delamination. We model the delamination as a thin opening between two materials of different acoustic properties, and using asymptotic techniques we derive a asymptotic model where the delaminated region is replaced by jump conditions on the acoustic field and flux. The asymptotic model has potential singularities due to the edges of the delaminated region, and we show that the forward problem is well posed for a large class of possible delaminations. We then design a special Linear Sampling Method (LSM) for detecting the shape of the delamination assuming that the background, undamaged, state is known. Finally we show, by numerical experiments, that our LSM can indeed determine the shape of delaminated regions.

7.2. Shape and topology optimization

7.2.1. Second-order shape derivatives along normal trajectories, governed by Hamilton-Jacobi equations

G. Allaire, E. Cancès and J.-L. Vié

In this work we introduce a new variant of shape differentiation which is adapted to the deformation of shapes along their normal direction. This is typically the case in the level-set method for shape optimization where the shape evolves with a normal velocity. As all other variants of the orginal Hadamard method of shape differentiation, our approach yields the same first order derivative. However, the Hessian or second-order derivative is different and somehow simpler since only normal movements are allowed. The applications of this new Hessian formula are twofold. First, it leads to a novel extension method for the normal velocity, used in the Hamilton-Jacobi equation of front propagation. Second, as could be expected, it is at the basis of a Newton optimization algorithm which is conceptually simpler since no tangential displacements have to be considered. Numerical examples are given to illustrate the potentiality of these two applications. The key technical tool for our approach is the method of bicharacteristics for solving Hamilton-Jacobi equations. Our new idea is to differentiate the shape along these bicharacteristics (a system of two ordinary differential equations).

7.2.2. Introducing a level-set based shape and topology optimization method for the wear of composite materials with geometric constraints

G. Allaire, F. Feppon, G. Michailidis, M.S. Sidebottom, B.A. Krick and N. Vermaak

The wear of materials continues to be a limiting factor in the lifetime and performance of mechanical systems with sliding surfaces. As the demand for low wear materials grows so does the need for models and methods to systematically optimize tribological systems. Elastic foundation models offer a simplified framework to study the wear of multimaterial composites subject to abrasive sliding. Previously, the evolving wear profile has been shown to converge to a steady-state that is characterized by a time-independent elliptic equation. In this article, the steady-state formulation is generalized and integrated with shape optimization to improve the wear performance of bi-material composites. Both macroscopic structures and periodic material microstructures are considered. Several common tribological objectives for systems undergoing wear are identified and mathematically formalized with shape derivatives. These include (i) achieving a planar wear surface from multimaterial composites and (ii) minimizing the run-in volume of material lost before steady-state wear is achieved. A level-set based topology optimization algorithm that incorporates a novel constraint on the level-set function is presented. In particular, a new scheme is developed to update material interfaces; the scheme (i) conveniently enforces volume constraints at each iteration, (ii) controls the complexity of design features using perimeter penalization, and (iii) nucleates holes or inclusions with the topological gradient. The broad applicability of the proposed formulation for problems beyond wear is discussed, especially for problems where convenient control of the complexity of geometric features is desired.

7.2.3. Geometric constraints for shape and topology optimization in architectural design

G. Allaire, C. Dapogny, A. Faure, G. Michailidis, A. Couvelas and R. Estevez

This work proposes a shape and topology optimization framework oriented towards conceptual architectural design. A particular emphasis is put on the possibility for the user to interfere on the optimization process by supplying information about his personal taste. More precisely, we formulate three novel constraints on the geometry of shapes; while the first two are mainly related to aesthetics, the third one may also be used to handle several fabrication issues that are of special interest in the device of civil structures. The common mathematical ingredient to all three models is the signed distance function to a domain, and its sensitivity analysis with respect to perturbations of this domain; in the present work, this material is extended to the case where the ambient space is equipped with an anisotropic metric tensor. Numerical examples are discussed in two and three space dimensions.

7.2.4. Modal basis approaches in shape and topology optimization of frequency response problems

G. Allaire and G. Michailidis

The optimal design of mechanical structures subject to periodic excitations within a large frequency interval is quite challenging. In order to avoid bad performances for non-discretized frequencies, it is necessary to finely discretize the frequency interval, leading to a very large number of state equations. Then, if a standard adjoint-based approach is used for optimization, the computational cost (both in terms of CPU and memory storage) may be prohibitive for large problems, especially in three space dimensions. The goal of the present work is to introduce two new non-adjoint approaches for dealing with frequency response problems in shape and topology optimization. In both cases, we rely on a classical modal basis approach to compute the states, solutions of the direct problems. In the first method, we do not use any adjoint but rather directly compute the shape derivatives of the eigenmodes in the modal basis. In the second method, we compute the adjoints of the standard approach by using again the modal basis. The numerical cost of these two new strategies are much smaller than the usual ones if the number of modes in the modal basis is much smaller than the number of discretized excitation frequencies. We present numerical examples for the minimization of the dynamic compliance in two and three space dimensions.

7.3. Direct scattering problems

7.3.1. Finite element methods for eigenvalue problems with sign-changing coefficients

C. Carvalho, P. Ciarlet and L. Chesnel

We consider a class of eigenvalue problems involving coefficients changing sign on the domain of interest. We analyse the main spectral properties of these problems according to the features of the coefficients. Under some assumptions on the mesh, we study how one can use classical finite element methods to approximate the spectrum as well as the eigenfunctions while avoiding spurious modes. We also prove localisation results of the eigenfunctions for certain sets of coefficients.

7.3.2. A Volume integral method for solving scattering problems from locally perturbed periodic layers

H. Haddar and T.P. Nguyen

We investigate the scattering problem for the case of locally perturbed periodic layers in R^d, $d = 2, 3$. Using the Floquet-Bloch transform in the periodicity direction we reformulate this scattering problem as an equivalent system of coupled volume integral equations. We then apply a spectral method to discretize the obtained system after periodization in the direction orthogonal to the periodicity directions of the medium. The convergence of this method is established and validating numerical results are provided.

7.4. Asymptotic Analysis

7.4.1. Small obstacle asymptotics for a non linear problem

L. Chesnel, X. Claeys and S.A. Nazarov

We study a 2D semi-linear equation in a domain with a small Dirichlet obstacle of size δ. Using the method of matched asymptotic expansions, we compute an asymptotic expansion of the solution as δ tends to zero. Its relevance is justified by proving a rigorous error estimate. We also construct an approximate model, based on an equation set in the limit domain without the small obstacle, which provides a good approximation of the far field of the solution of the original problem. The interest of this approximate model lies in the fact that it leads to a variational formulation which is very simple to discretize. We present numerical experiments to illustrate the analysis.

7.4.2. Influence of the geometry on plasmonic waves

L. Chesnel X. Claeys and S.A. Nazarov

In the modeling of plasmonic technologies in time harmonic regime, one is led to study the eigenvalue problem $-\div(\sigma\nabla u) = \lambda u$ (P), where σ is a physical coefficient positive in some region Ω_+ and negative in some other region Ω_-. We highlight an unusual instability phenomenon for the source term problem associated with (P): for certain configurations, when the interface between Ω_+ and Ω_- presents a rounded corner, the solution may depend critically on the value of the rounding parameter. We explain this property studying the eigenvalue problem (P). We provide an asymptotic expansion of the eigenvalues and prove error estimates. We establish an oscillatory behaviour of the eigenvalues as the rounding parameter of the corner tends to zero. These theoretical results are illustrated by numerical experiments.

7.4.3. Instability of dielectrics and conductors in electrostatic fields

G. Allaire and J. Rauch

This work proves most of the assertions in section 116 of Maxwell's treatise on electromagnetism. The results go under the name Earnshaw's Theorem and assert the absence of stable equilibrium configurations of conductors and dielectrics in an external electrostatic field.

7.4.4. Optimization of dispersive coefficients in the homogenization of the wave equation in periodic structures

G. Allaire and T. Yamada

We study dispersive effects of wave propagation in periodic media, which can be modelled by adding a fourth-order term in the homogenized equation. The corresponding fourth-order dispersive tensor is called Burnett tensor and we numerically optimize its values in order to minimize or maximize dispersion. More precisely, we consider the case of a two-phase composite medium with an 8-fold symmetry assumption of the periodicity cell in two space dimensions. We obtain upper and lower bound for the dispersive properties, along with optimal microgeometries.

7.4.5. Homogenization of Stokes System using Bloch Waves

G. Allaire, T. Ghosh and M. Vanninathan

In this work, we study the Bloch wave homogenization for the Stokes system with periodic viscosity coefficient. In particular, we obtain the spectral interpretation of the homogenized tensor. The presence of the incompressibility constraint in the model raises new issues linking the homogenized tensor and the Bloch spectral data. The main difficulty is a lack of smoothness for the bottom of the Bloch spectrum, a phenomenon which is not present in the case of the elasticity system. This issue is solved in the present work, completing the homogenization process of the Stokes system via the Bloch wave method.

7.5. Diffusion MRI

7.5.1. Adapting the Kärger model to account for finite diffusion-encoding pulses in diffusion MRI

H. Haddar, J.R. Li and S. Schiavi

Diffusion magnetic resonance imaging (dMRI) is an imaging modality that probes the diffusion characteristics of a sample via the application of magnetic field gradient pulses. If the imaging voxel can be divided into different Gaussian diffusion compartments with inter-compartment exchange governed by linear kinetics, then the dMRI signal can be described by the Kärger model, which is a well-known model in NMR. However, the Kärger model is limited to the case when the duration of the diffusion-encoding gradient pulses is short compared to the time delay between the start of the pulses. Under this assumption, the time at which to evaluate the Kärger model to obtain the dMRI signal is unambiguously the delay between the pulses. Recently, a new model of the dMRI signal, the Finite-Pulse Kärger (FPK) model, was derived for arbitrary diffusion gradient profiles. Relying on the FPK model, we show that when the duration of the gradient pulses is not short, the time at which to evaluate the Kärger model should be the time delay between the start of the pulses, shortened by one third of the pulse duration. With this choice, we show the sixth order convergence of the Kärger model to the FPK model in the non-dimensionalized pulse duration.

7.5.2. A macroscopic model for the diffusion MRI signal accounting for time-dependent diffusivity

H. Haddar, J.R. Li and S. Schiavi

An important quantity measured in dMRI in each voxel is the Apparent Diffusion Coefficient (ADC) and it is well-established from imaging experiments that, in the brain, *in-vivo*, the ADC is dependent on the measured diffusion time. To aid in the understanding and interpretation of the ADC, using homogenization techniques, we derived a new asymptotic model for the dMRI signal from the Bloch-Torrey equation governing the water proton magnetization under the influence of diffusion-encoding magnetic gradient pulses. Our new model was obtained using a particular choice of scaling for the time, the biological cell membrane permeability, the diffusion-encoding magnetic field gradient strength, and a periodicity length of the cellular geometry. The ADC of the resulting model is dependent on the diffusion time. We numerically validated this model for a wide range of diffusion times for two dimensional geometrical configurations.

7.5.3. Quantitative DLA-based Compressed Sensing for MEMRI Acquisitions

P. Svehla, K.-V. Nguyen, J.-R. Li and L. Ciobanu

High resolution Manganese Enhanced Magnetic Resonance Imaging (MEMRI) has great potential for functional imaging of live neuronal tissue at single neuron scale. However, reaching high resolutions often requires long acquisition times which can lead to reduced image quality due to sample deterioration and hardware instability. Compressed Sensing (CS) techniques offer the opportunity to significantly reduce the imaging time. The purpose of this work is to test the feasibility of CS acquisitions based on Diffusion Limited Aggregation (DLA) sampling patterns for high resolution quantitative MEMRI imaging. Fully encoded and DLA-CS MEMRI images of Aplysia californica neural tissue were acquired on a 17.2T MRI system. The MR signal corresponding to single, identified neurons was quantified for both versions of the T1 weighted images. Results: For a 50% undersampling, DLA-CS leads to signal intensity differences, measured in individual neurons, of approximately 1.37% when compared to the fully encoded acquisition, with minimal impact on image spatial resolution. At the undersampling ratio of 50%, DLA-CS is capable of accurately quantifying signal intensities in MEMRI acquisitions. Depending on the image signal to noise ratio, higher undersampling ratios can be used to further reduce the acquisition time in MEMRI based functional studies of living tissues.

7.5.4. The time-dependent diffusivity in the abdominal ganglion of Aplysia californica, comparing experiments and simulations

K.-V. Nguyen, D. Le Bihan, L. Ciobanu and J.-R. Li

The nerve cells of the *Aplysia* are much larger than mammalian neurons. Using the *Aplysia* ganglia to study the relationship between the cellular structure and the diffusion MRI signal can shed light on this relationship for more complex organisms. We measured the dMRI signal at several diffusion times in the abdominal ganglion and performed simulations of water diffusion in geometries obtained after segmenting high resolution T2-weighted images and incorporating known information about the cellular structure from the literature. By fitting the experimental signal to the simulated signal for several types of cells in the abdominal ganglion at a wide range of diffusion times, we obtained estimates of the intrinsic diffusion coefficient in the nucleus and the cytoplasm. We also evaluated the reliability of using an existing formula for the time-dependent diffusion coefficient to estimate cell size.

7.5.5. A two pool model to describe the IVIM cerebral perfusion

G. Fournet, J.-R. Li, A.M. Cerjanic, B.P. Sutton, L. Ciobanu and D. Le Bihan

IntraVoxel Incoherent Motion (IVIM) is a magnetic resonance imaging (MRI) technique capable of measuring perfusion-related parameters. In this manuscript, we show that the mono-exponential model commonly used to process IVIM data might be challenged, especially at short diffusion times. Eleven rat datasets were acquired at 7T using a diffusion-weighted pulsed gradient spin echo sequence with b-values ranging from 7 to 2500 s/mm^2 at 3 diffusion times. The IVIM signals, obtained by removing the diffusion component from the raw MR signal, were fitted to the standard mono-exponential model, a bi-exponential model and the Kennan model. The Akaike information criterion used to find the best model to fit the data demonstrates that, at short diffusion times, the bi-exponential IVIM model is most appropriate. The results obtained by comparing the experimental data to a dictionary of numerical simulations of the IVIM signal in microvascular networks support the hypothesis that such a bi-exponential behavior can be explained by considering the contribution of two vascular pools: capillaries and somewhat larger vessels.

7.5.6. The influence of acquisition parameters on the metrics of the bi-exponential IVIM model

G. Fournet, J.-R. Li, D. Le Bihan and L. Ciobanu

The IntraVoxel Incoherent Motion (IVIM) MRI signal, typically described as a mono-exponential decay, can sometimes be better modeled as a bi-exponential function accounting for two vascular pools, capillaries and medium-size vessels. The goal of this work is to define precisely in which conditions the IVIM signal shape becomes bi-exponential and to understand the evolution of the IVIM outputs with different acquisition parameters. Rats were scanned at 7T and 11.7T using diffusion-weighted pulsed-gradient spin-echo (SE) and stimulated-echo (STE) sequences with different repetition times (TR) and diffusion encoding times. The obtained IVIM signals were fit to the mono- and bi-exponential models and the output parameters compared. The bi-exponential and mono-exponential models converge at long diffusion encoding times and long TRs. The STE is less sensitive to inflow effects present at short TRs, leading to a smaller volume fraction for the fast pool when compared to the SE sequence. The two vascular components are more easily separated at short diffusion encoding times, short TRs and when using a SE sequence. The volume fractions of the two blood pools depend on the pulse sequence, TR and diffusion encoding times while the pseudo-diffusion coefficients are only affected by the diffusion encoding time.

ECUADOR Project-Team

6. New Results

6.1. AD-adjoints and C dynamic memory management

Participants: Laurent Hascoët, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)], Mathieu Morlighem [University of California at Irvine (USA)].

One of the current frontiers of AD research is the definition of an adjoint AD model that can cope with dynamic memory management. This research is central in our ongoing effort towards adjoint AD of C, and more remotely towards AD of C++. This research is conducted in collaboration with the MCS department of Argonne National Lab. Our partnership is formalized by joint participation in the Inria joint lab JLESC, and partly funded by the Partner University Fund (PUF) of the French embassy in the USA.

Adjoint AD must reproduce in reverse order the control decisions of the original code. In languages such as C, allocation of dynamic memory and pointer management form a significant part of these control decisions. Reproducing memory allocation in reverse means reallocating memory, possibly receiving a different memory chunk. Reproducing pointer addresses in reverse thus require to convert addresses in the former memory chunks into equivalent addresses in the new reallocated chunks. Together with Krishna Narayanan from Argonne, we experiment on real applications to find the most efficient solution to this address conversion problem. We jointly develop a library (called ADMM, ADjoint Memory Management) whose primitives are used in AD adjoint code to handle this address conversion. Both our AD tool Tapenade and Argonne's tool OpenAD use ADMM in the adjoint code they produce.

This year, ADMM was instrumental in the successful generation of the adjoint code of "ALIF" (formerly called "SEISM") by Tapenade. The "ALIF" code is developed by Mathieu Morlighem from UC Irvine, jointly with Eric Larour from JPL. This glaciology code is a C clone of the C++ "ISSM" code from JPL. One objective of this work is to clarify the C programming style that allows AD to perform better. Another objective is to make progress in the direction of generating adjoints of C++ code. Although ADMM has already been used with success for the adjoint of several small- to medium-size applications, and now on the large-size code "ALIF", we are still considering alternative implementation strategies. This work was presented at the AD2016 conference in Oxford [16], and an article is submitted to journal "Optimization Methods and Software".

6.2. AD-adjoints of MPI-parallel codes

Participants: Laurent Hascoët, Ala Taftaf, Georgios Ntanakas [Rolls-Royce, Dahlewitz, Germany], Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)].

We have a long-standing collaboration with Argonne National Lab on the question of adjoint AD of message-passing parallel codes. We continued joint development of the Adjoinable-MPI library (AMPI) that provides efficient tangent and adjoint AD for MPI-parallel codes, independently of the AD tool used (now AdolC, dco, OpenAD, Tapenade).

Ala Taftaf considers the question of checkpointing applied to the AD-adjoint of an MPI-parallel code. Checkpointing is a memory/runtime tradeoff which is essential for adjoint AD of large codes, in particular parallel codes. However, for MPI codes this question has always been addressed by ad-hoc hand manipulations of the differentiated code, and with no formal assurance of correctness. Ala Taftaf studies these past experiments and proposes more general strategies. Ala Taftaf presented her results [20], [23] at the Eccomas 2016 conference (Crete) in June and at the NOED 2016 conference (Munich) in july [22].

During his secondment with our team, PhD student Georgios Ntanakas from Rolls-Royce studied possible extension of Tapenade to handle the parallel constructs in Rolls-Royce's "Hydra" code, which rely on a special parallel library named "OPlus".

6.3. AD-adjoints of Iterative Processes

Participants: Laurent Hascoët, Ala Taftaf, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)], Daniel Goldberg [University of Edinburgh, UK].

Ala Taftaf continued her work on the adjoint of iterative Fixed-Point loops. This year she studied refinements of the AD-specific data-flow analyses to adapt them to the specific shape of this adjoint code, proposed by Bruce Christianson [27]. She also proposed an efficient "warm-start" mechanism, that provides a good initial guess for the fixed-point loop that computes the adjoint, in the case where this fixed-point loop is itself enclosed in another loop. These results are described in her PhD document, to be defended in January 2017.

We published a journal article [13] on our joint work with Krishna Narayanan from ANL and Dan Goldberg from University of Edinburgh (UK), which applies in particular this fixed-point adjoint strategy to a glaciology configuration of the MIT GCM code.

6.4. AD of mixed-language codes

Participants: Valérie Pascual, Tom Verstraete [VKI, Brussels, Belgium], Laurent Hascoët.

In collaboration with Tom Verstraete, Valérie Pascual is applying Tapenade to the library "Calculix", whose implementation mixes Fortran and C. This library is well fit for Tapenade differentiation, as the internal representation that we use for codes is language-independent. We can thus load both Fortran and C source into Tapenade and differentiate the complete code transparently. Obviously, since this is the first application of Tapenade to a real-size mixed-language code, interesting problems arise mostly about parameter-passing strategies. Valérie Pascual presented her first results at the AD2016 conference in Oxford [21].

6.5. Multirate methods

Participants: Alain Dervieux, Bruno Koobus, Emmanuelle Itam, Stephen Wornom.

This study is performed in collaboration with IMAG-Montpellier II. It addresses an important complexity issue in unsteady mesh adaptation and takes place in the work done in the ANR Maidesc. Unsteady high-Reynolds computations are strongly penalized by the very small time-step imposed by accuracy requirements on regions involving small space-time scales. Unfortunately, this is also true for sophisticated unsteady mesh adaptive calculations. This small time-step is an important computational penalty for mesh adaptive methods of AMR type. This is also the case for the Unsteady Fixed-Point mesh-adaptive methods developed by Ecuador in cooperation with the Gamma3 team of Inria-Saclay. In the latter method, the loss of efficiency is even more crucial when the anisotropic mesh is locally strongly streched. This loss is evaluated as limiting the numerical convergence order for discontinuities to 8/5 instead of second-order convergence. An obvious remedy is to design time-consistent methods using different time steps on different parts of the mesh, as far as they are efficient and not too complex. The family of time-advancing methods in which unsteady phenomena are computed with different time steps in different regions is referred to as the multirate methods. In our cooperation with university of Montpellier, a novel multirate method using cell agglomeration has been designed and developed in our AIRONUM CFD platform. A series of large-scale test cases show that the new method is much more efficient than an explicit method, while retaining a similar time accuracy over the whole computational domain. The comparison with an implicit scheme shows that the implicit scheme is in some cases one order less accurate due to higher time steps and higher dissipation. A communication has been presented at ECCOMAS [17] and an article is submitted to a journal.

6.6. Application of AD to uncertainties and errors in CFD

Participants: Valérie Pascual, Laurent Hascoët, Alain Dervieux.

An important application of AD is the creation of uncertainty management tools, as first and second derivatives are used for the assembly of perturbation-based models for Uncertainty Quantification.

During the FP7 project UMRIDA, finished in september 2016, Inria has assisted Alenia-Aermacchi and WUT (Warsaw) in applying Tapenade to a CFD software for perturbation-based models.

We contributed the following chapters to the UMRIDA monography [24]:

- II.5.0 Introduction to Intrusive Perturbation Methods
- II.5.1 Algorithmic Differentiation for second derivatives
- III.a.4 Introduction to Intrusive Perturbation Methods and their range of applicability
- IV.3 Use of Automatic Differentiation tools at the example of Tapenade

6.7. Control of approximation errors

Participants: Gautier Brèthes, Eléonore Gauci, Alain Dervieux, Adrien Loseille [Gamma3 team, Inria-Rocquencourt], Frédéric Alauzet [Gamma3 team, Inria-Rocquencourt], Loïc Frazza [Gamma3 team, Inria-Saclay], Stephen Wornom, Anca Belme [university of Paris 6].

Reducing approximation errors as much as possible is a particular kind of optimal control problem. We formulate it exactly this way when we look for the optimal metric of the mesh, which minimizes a user-specified functional (goal-oriented mesh adaptation). In that case, the usual methods of optimal control apply, using adjoint states that can be produced by Algorithmic Differentiation.

Our theoretical studies in mesh adaptation are supported by the ANR project MAIDESC coordinated by ECUADOR and Gamma3, which deals with meshes for interfaces, third-order accuracy, meshes for boundary layers, and curved meshes.

The thesis of Éléonore Gauci on the goal-oriented criteria for CFD and coupled CSM-CFD systems is continuing. Éléonore Gauci gave a presentation at ECCOMAS in Crete.

Further studies of mesh adaptation for viscous flows are currently performed and a paper in collaboration with Gamma3 and university of Paris 6 (Anca Belme) is being written for a Journal.

An important novelty in mesh adaption is the norm-oriented AA method. The method relies on the definition of ad hoc correctors. It has been developed in the academic platform "FMG" for elliptic problems. Gautier Brèthes gave several presentations in conferences, a journal article has been published [12]. The introduction of the norm-oriented idea considerably amplifies the impact of adjoint-based AA. The applied mathematician and the engineer now have methods when faced to mesh adaptation for the simulation of a complex PDE system, since they can specify which error norm level they wish, and for which norm. Another version is developed jointly with Inria team Gamma3 for the compressible Euler model.

A work of extension of a different standpoint, the tensorial metric method was started during the thesis of Gautier Brèthes and has been been submitted to a journal.

CFD application are supported by the European FP7 project UMRIDA which deals with the application of AA to approximation error modelling and control.

This involves an extensive work on a series of RANS (Reynolds Averaged Navier-Stokes) adaptative computations relying on the multi-scale method on the one hand, and on the other hand on further development by Gamma3 and Ecuador of the novel norm-oriented method for the compressible Euler model. This will be first published as a chapter contributed to the UMRIDA monography [24]: II.1.4 Numerical uncertainties estimation and mitigation by mesh adaption Frédéric Alauzet, Alain Dervieux, Loïc Frazza and Adrien Loseille.

6.8. Turbulence models

Participants: Alain Dervieux, Bruno Koobus, Emmanuelle Itam, Marianna Braza [CNRS-IMFT at Toulouse], Stephen Wornom, Bruno Sainte-Rose [Lemma].

Modeling turbulence is an essential aspect of CFD. The purpose of our work in hybrid RANS/LES (Reynolds Averaged Navier-Stokes / Large Eddy Simulation)is to develop new approaches for industrial applications of LES-based analyses. In the applications targetted (aeronautics, hydraulics), the Reynolds number can be as high as several tenth millions, far too high for pure LES models. However, certain regions in the flow can be better predicted with LES than with usual statistical RANS (Reynolds averaged Navier-Stokes) models. These are mainly vortical separated regions as assumed in one of the most popular hybrid model, the hybrid Detached Eddy Simulation model. Here, "hybrid" means that a blending is applied between LES and RANS. An important difference between a real life flow and a wind tunnel or basin is that the turbulence of the flow upstream of each body is not well known.

This year, we have validated and experimented for various test cases the integration of the boundary layer by adding the so-called Menter correction imposing the Bradshaw law. We have studied these improvements on multiple-body flows. An emblematic case is the interaction between two parallel cylinders, one being in the wake of the other.

The development of hybrid models, in particular DES in the litterature has raised the question of the domain of validity of these models. According to theory, these models should not be applied to flow involving laminar boundary layers (BL). But industrial flows are complex flows and often present regions of laminar BL, regions of fully developed turbulent BL and regions of non-equilibrium vortical BL. It is then mandatory for industrial use that the new hybrid models give a reasonable prediction for all these types of flow. This year, we concentrated on evaluating the behavior of hybrid models for laminar BL and for vortical wakes. While less predictive than pure LES on laminar BL, some hybrid models still give reasonable predictions for rather low Reynolds numbers. A little surprisingly, the prediction of vortical wakes needs some improvement. For this improvement, we propose a hybrid formulation involving locally a sophisticated LES-VMS (Large Eddy Simulation - Variational Multi-Scale) model combined with the dynamic local limitation of Germano-Piomelli. Several standard options together with the new model have been compared for a series of test cases: a communication has been presented in a conference [18] and an article is in preparation.

GAMMA3 Project-Team

4. New Results

4.1. Remaillage adaptatif pour la mise en forme de tôles minces et de composites

Participants: Laurence Moreau [correspondant], Abel Cherouat, Houman Borouchaki.

Au cours des simulations numériques de mise en forme en 3D, les grandes déformations mises en jeu font que le maillage subit de fortes distorsions. Il est alors nécessaire de remailler continuellement la pièce afin de pouvoir capturer les détails géométriques des surface en contact, adapter la taille du maillage à la solution physique et surtout pouvoir effectuer la simulation jusqu'à la fin du procédé de mise en forme. Lorsque la pièce est comprise entre des outils rigides (cas de l'emboutissage), aux problèmes de remaillage s'ajoutent aussi des difficultés sur la gestion du contact entre les pièces. Une méthode couplant une stratégie de remaillage adaptatif et une technique de projection a été développée. Afin de pouvoir réaliser des simulations numériques de composites tissés, une procédure spécifique a été ajoutée au remailleur afin de pouvoir raffiner les éléments finis bi-composants (association d'éléments finis de barre et de membrane orientés matérialisant le comportement de fibres chaîne et trame).

Ce travail a donnée lieu à 1 article.

4.2. Le formage incrémental : étude expérimentale, numérique et remaillage adaptatif

Participants: Laurence Moreau [correspondant], Abel Cherouat, Houman Borouchaki.

Le formage incrémental est un procédé de mise en forme récent permettant de mettre en forme des tôles minces grâce au déplacement d'un outil hémisphérique dont la trajectoire est pilotée par une machine à commande numérique. Ce procédé peu couteux est une alternative intéressante à l'emboutissage traditionnel pour les entreprises réalisant des pièces de petite taille à usage unique ou en petite série comme les entreprises biomédicales (prothèses, implants personnalisés..). Cependant, il reste encore des développements importants sur le plan numérique et expérimental pour que ce procédé soit industrialisable : problèmes d'état de surface, de non-respect de la géométrie, risques de rupture. Nous avons étudié numériquement et expérimentalement ce procédé de formage incrémental : développement d'une méthode de remaillage adaptée à ce procédé, optimisation des paramètres du procédé, étude du formage incrémental à chaud, étude du formage incrémental robotisé.r

Ce travail a donnée lieu à 2 articles et 5 participations à des conférences internationales.

4.3. Reconstruction de surface 3D à partir d'images numériques 2D

Participants: Laurence Moreau [correspondant], Abel Cherouat, Houman Borouchaki.

Ces travaux portent sur la reconstruction 3D d'objets à partir de plusieurs photos prises via des caméras calibrées avec des points de vue différents couvrant la totalité de la surface de l'objet. La méthodologie générale consiste à apparier les pixels correspondants de deux photos et obtenir des positions 3D via une technique de triangulation.. L'idée originale réside dans une nouvelle méthodologie automatique d'appariement de pixels. Elle comprend trois étapes : un motif présentant un maillage triangulaire aléatoire est projeté sur l'objet 3D, le maillage est identifié sur chaque photo et la technique de triangulation est appliquée aux sommets de ce maillage. La méthodologie de reconstruction 3D a été appliquée à la modélisation géométrique du buste féminin afin d'envisager des simulations de comportements statique et dynamique de ce buste. Ces travaux ont conduit aussi à la conception et la réalisation d'une cabine d'acquisition permettant de prendre 24 prises de vue de manière simultanée depuis un ordinateur extérieur à la cabine.

Ce travail a donnée lieu à 1 article et 2 participations à des conférences internationales.

4.4. Modélisation numérique, remaillage adaptatif et optimisation pour la morphologie de nanofils

Participants: Laurence Moreau [correspondant], Thomas Grosges.

L'objectif était de développer une méthode permettant de détecter et d'analyser la présence de nanomatériaux dans l'eau. Une voie possible consiste à étudier les effets liés aux couplages lumière-matière, c'est-à-dire la réponse photo-thermique des nanomatériaux illuminés par une onde électromagnétique. La méthode proposée consiste à étudier la réponse thermique du nanofil immergé sous l'illumination et à la relier à la bulle produite. Le problème multi physique est modélisé par un système d'équations couplées : équation de Helmoltz et équation de la chaleur. La résolution numérique de ces équations est effectuée par une méthode des éléments finis et un processus d'optimisation incluant des boucles de remaillages adaptatifs afin de contrôler la précision de la solution et assurer la convergence. Une étude de la morphologie de la bulle a été réalisée en fonction de paramètres géométriques et physiques. Deux fonctions permettant de relier la taille de la bulle à la taille et la forme du nanomatériau ont été définies. La résolution du modèle inverse, associé à ces fonctions, permettant de remonter à la morphologie du nanomatériau via celle de la bulle. L'efficacité et la pertinence du modèle ont été montrées en confrontant les résultats numériques aux résultats expérimentaux.

Ce travail a donnée lieu à 3 articles et 2 participations à des conférences internationales

4.5. Les outils de remaillage dans la simulation multi-physiques pour la fiabilisation des systèmes complexes

Participants: Abel Cherouat [correspondant], Houman Borouchaki.

Le projet concerne la maîtrise des outils de simulation numérique multi-physique avec remaillage adaptatif 3D pour la prévention de la fiabilité des systèmes complexes. Les systèmes étudiés sont des structures comportant des composants et des architectures mécaniques. Ils sont fortement contraints car la partie électro-magnétique est très sensible aux vibrations, variations et dilatations thermiques, et agressions physico-chimiques qui existent habituellement dans les systèmes mécaniques. La fiabilisation représente des enjeux majeurs pour ces systèmes. L'objectif final est d'étudier la fiabilisation de ces systèmes par des approches hybrides qui combinent les outils de simulation éléments finis multi-physiques couplées avec adaptation en temps réel des maillages éléments finis en 3D. L'analyse de la fiabilité et la synthèse pouvant être appliquées en cas de défaillance pour maintenir l'exploitation des systèmes.

Ce travail a donnée lieu à 4 articles et 2 participations à des conférences internationales.

4.6. Les matériaux innovants : mousses métalliques - AMF, textiles techniques, composites et agro-composites : Modélisation mécanique, Simulation avec remaillage, Reconstitution 3D et Modélisation géométrique

Participants: Abel Cherouat [correspondant], Houman Borouchaki, Shijie Zhu, Antony Sheedev.

Le contexte de l'étude sur les mousses est la modélisation du comportement mécanique, la reconstitution 3D de la morphologie des mousses à partir d'images tomographiques ou de la CAO géométrique, de l'optimisation et de la simulation de la déformation de mousse (métalliques ou AMF).

Le contexte de l'étude sur les agro-composites est la maitrise des matières naturelles, l'allégement des structures et la valorisation de l'émergence des textiles biodégradables pour des applications industrielles. Les investigations concernent les aspects d'élaboration et mise en œuvre des textiles secs ou pré-imprégnés (tissés, UD cousu et mats), de caractérisation-modélisation comportementale multi-échelle et de mise au point d'outils d'aide à la décision et d'éco-conception des matériaux fonctionnels.

Le contexte de l'étude sur les composites est l'éco-réparation *in-situ* des structures industrielles intégrant l'hybridation de procédés émergents d'*additive manufacturing* et le frittage micro-onde avec l'utilisation de nouvelles résines ou nuances de matériaux, la numérisation 3D, l'impression ou collage par balayage et le contrôle non destructif.

Le contexte de l'étude sur les tissus biologiques est le développement de méthode d'obtention des paramètres mécaniques des tissus vivants et des informations pour l'amélioration des prothèses post-chirurgicale (un sein artificiel). Une approche médicale de la modélisation du sein et de sa déformabilité a pour objectif de prédire les déformations des tissus pendant les interventions en tenant compte des constituants (graisses, glandes, peau et ligaments), mais ne concerne pas le comportement du sein et son remodelage par le bonnet ou son comportement pendant le sport.

Ce travail a donnée lieu à 11 articles et 8 participations à des conférences internationales.

4.7. Reconstruction 3D à partir d'image vs Scanner 3D, Maillage adaptatif par vision embarquée sur drones autonomes

Participants: Abel Cherouat [correspondant], Houman Borouchaki.

Dans le cadre de ce projet, on se propose de concevoir un système de reconstruction adaptative et temps réel de scènes 3D en se basant uniquement sur le flux d'images captées par une caméra embarquée sur un drone autonome. Un nuage de points peut être ainsi obtenu en traitant d'une manière efficace et temps-réel le flux d'images issues de la caméra mobile. Le nuage de points en temps réel est utilisé pour reconstruire les surfaces des objets constituant la scène, et surtout de quantifier la qualité de la reconstruction en fonction de la géométrie de ces surfaces. Les applications concernées sont les automates industriels, l'imagerie médicale, le *Smart Tracking*, la surveillance et la sécurité, la rétro-conception et la réalité augmentée, ...

Ce travail a donnée lieu à 2 articles et 2 participations à des conférences internationales.

4.8. Les outils de remaillage dans la simulation et l'optimisation de la mise en forme des matériaux

Participants: Abel Cherouat [correspondant], Houman Borouchaki, Laurence Moreau.

L'objectif scientifique de ce projet est de développer des modèles théoriques, numériques et géométriques nécessaires à la mise au point de méthodologies de simulation numérique et d'optimisation de procédés de fabrication et de mise en forme de composants et de structures mécaniques en petites ou en grandes déformations. Une attention particulière est accordée à la génération de maillage, de remaillage et de maillage adaptatif isotrope et anisotrope plan (2D), surfacique (2,5D) et volumique (3D), ainsi que des méthodes d'optimisation de maillages (en particulier surfacique) ainsi que les couplages multi-physiques entre les différents phénomènes.

Ce travail a donnée lieu à 13 articles et 4 participations à des conférences internationales.

4.9. Applications du maillage et développements de méthodes avancées pour la cryptographie

Participants: Thomas Grosges [correspondant], Dominique Barchiesi, Michael François.

L'utilisation des nombres (pseudo)-aléatoires a pris une dimension importante ces dernières décennies. De nombreuses applications dans le domaine des télécommunications, de la cryptographie, des simulations numériques ou encore des jeux de hasard, ont contribué au développement et à l'usage de ces nombres. Les méthodes utilisées pour la génération de tels nombres (pseudo)-aléatoires proviennent de deux types de processus : physique et algorithmique. Ce projet de recherche a donc pour objectif principal le développement de nouveaux procédés de génération de clés de chiffrement, dits “exotiques”, basés sur des processus physiques, multi-échelles, multi-domaines assurant un niveau élevé de sécurité. Deux classes de générateurs basés sur des principes de mesures physiques et des processus mathématiques ont été développé.

La première classe de générateurs exploite la réponse d'un système physique servant de source pour la génération des séquences aléatoires. Cette classe utilise aussi bien des résultats de simulations que des résultats de mesures interférométriques pour produire des séquences de nombres aléatoires. L'application du maillage adaptatif sert au contrôle de l'erreur sur la solution des champs physiques (simulés ou mesurés). À partir de ces cartes physiques, un maillage avec estimateur d'erreur sur l'entropie du système est appliqué. Celui-ci permet de redistribuer les positions spatiales des noeuds. L'étude (locale) de la réduction d'entropie des clés tout au long de la chaîne de création et l'étude (globale) de l'entropie de l'espace des clés générées sont réalisées à partir de tests statistiques.

La seconde classe de générateurs porte sur le développement de méthodes avancées et est basée sur l'exploitation de fonctions chaotiques en utilisant les sorties de ces fonctions comme indice de permutation sur un vecteur initial. Ce projet s'intéresse également aux systèmes de chiffrement pour la protection des données et deux algorithmes de chiffrement d'images utilisant des fonctions chaotiques sont développés et analysés. Ces algorithmes utilisent un processus de permutation-substitution sur les bits de l'image originale. Une analyse statistique approfondie confirme la pertinence des cryptosystèmes développés. Les résultats de cette recherche se sont vu récompensés par un premier prix décerné par EURASIP (European Association in Signal Processing) en 2016 ("Best paper award of the EURASIP).

4.10. Méthodes avancées pour la nanomorphologie des nanotubes/fils en suspension liquide"

Participants: Thomas Grosges [correspondant], Dominique Barchiesi, Abel Cherouat, Houman Borouchaki, Laurence Giraud-Moreau, Anis Chaari.
Validité du projet: 2011-2015.
Production scientifique: 1 thèse soutenue en 2016 (A. Chaari), 3 articles publiés, 1 conférence nternationale (PIERS 2014), 2 conférences nationales (CSMA 2013 et CSMA 2015).
Ce projet de recherche (NANOMORPH) a pour objet principal le développement et la mise au point d'une instrumentation optique pour déterminer la distribution en tailles et le coefficient de forme de nanofils (NF) ou de nanotubes (NT) en suspension dans un écoulement. Au cours de ce projet, deux types de techniques optiques complémentaires sont développées. La première, basée sur la diffusion statique de la lumière, nécessite d'étudier au préalable la physico-chimie de la dispersion, la stabilisation et l'orientation des nanofils dans les milieux d'étude. La seconde méthode, basée sur une méthode opto-photothermique pulsée, nécessite en sus, la modélisation de l'interaction laser/nanofils, ainsi que l'étude des phénomènes multiphysiques induits par ce processus. L'implication de l'équipe-projet GAMMA3 concerne principalement la simulation multiphysique de l'interaction laser-nanofils et l'évolution temporelle des bulles et leurs formations. L'une des principales difficultés de ces problématiques est que la géométrie du domaine est variable (à la fois au sens géométrique et topologique). Ces simulations ne peuvent donc être réalisées que dans un schéma adaptatif de calcul nécessitant le remaillage tridimensionnel mobile, déformable avec topologie variable du domaine (formation et évolution des bulles au cours du temps et de l'espace).

4.11. Méthodes de résolutions avancées et modélisation électromagnetisme-thermique-mécanique à l'échelle mesoscopique

Participants: Dominique Barchiesi [correspondant], Abel Cherouat, Thomas Grosges, Houman Borouchaki, Laurence Giraud-Moreau, Sameh Kessentini, Anis Chaari, Fadhil Mezghani
Validité du projet: 2009-2016 (thèse de Fadhil Mezghani initiée en 2012 coencadrée par D. Barchiesi et A. Cherouat).
Production scientifique: 2 thèses soutenues (S. Kessentini, 22/10/2012 et F. Mezghani), 15 articles publiés, 6 conférences.

Le contrôle et l'adaptation du maillage lors de la résolution de problèmes couplés et/ou non linéaires reste un problème ouvert et fortement dépendant du type de couplage physique entre les EDP à résoudre. Notre objectif est de développer des modèles stables afin de calculer les dilatations induites par l'absorption d'énergie électromagnétique, par des structures matérielles inférieures au micron. Les structures étudiées sont en particulier des nanoparticules métalliques en condition de résonance plasmon. Dans ce cas, un maximum d'énergie absorbée est attendu, accompagné d'un maximum d'élévation de température et de dilatation. Il faut en particulier développer des modèles permettant de simuler le comportement multiphysique de particules de formes quelconques, pour une gamme de fréquences du laser d'éclairage assez étendue afin d'obtenir une étude spectroscopique de la température et de la dilatation. L'objectif intermédiaire est de pouvoir quantifier la dilatation en fonction de la puissance laser incidente. Le calcul doit donc être dimensionné et permettre finalement des applications dans les domaines des capteurs et de l'ingénierie biomédicale. En effet, ces nanoparticules métalliques sont utilisées à la fois pour le traitement des cancers superficiels par nécrose de tumeur sous éclairage adéquat, dans la fenêtres de transparence cellulaire. Déposées sur un substrat de verre, ces nanoparticules permettent de construire des capteurs utilisant la résonance plasmon pour être plus sensibles (voir projet européen *Nanoantenna* et l'activité génération de nombres aléatoires). Cependant, dans les deux cas, il est nécessaire, en environnement complexe de déterminer la température locale, voire la dilatation de ces nanoparticules, pouvant conduire à un désaccord du capteur, la résonance plasmon étant très sensible aux paramètres géométriques et matériels des nanostructures. En ce sens, l'étude permet d'aller plus loin que la "simple" interaction électromagnétique avec la matière du projet européen *Nanoantenna*.

Le travail a constitué en la poursuite de l'étude des spécificités de ce type de problème multiphysique pour des structures de forme simple et la mise en place de fonctions test, de référence, pour les développements de maillage adaptatifs pour les modèles multiphysiques éléments finis. Nous espérons pouvoir proposer un projet ANR couplant les points de vue microscopiques et macroscopiques dans les prochaines années.

4.12. Problèmes de magnétostatique sur maillage de grande taille et multi-échelle

Participants: Dominique Barchiesi [correspondant], Thomas Grosges, Houman Borouchaki, Brahim Yahiaoui
Validité du projet: 2013-2015. Post-doc Brahin Yahiaoui.
Le projet Flyprod concerne l'étude du stockage d'électricité par volant d'inertie lévité et financé par l'ADEME. Une technologie brevetée innovante et stratégique permettant à des acteurs majeurs de la distribution électrique de stocker de l'énergie pour des périodes de fortes consommations. D'un point de vue écologique, un volant d'inertie n'émet ni gaz à effet de serre, ni produits chimiques nocifs pour l'environnement. Les partenaires pour ce projet sont LEVISYS, Université de Technologie de Troyes, SCLE SFE (COFELY INEO, Groupe GDFSUEZ), CIRTEM, Conseil Général de l'Aube. Les dispositifs mis en oeuvre nécessitent des études approfondies pour rendre les volants d'inertie économiquement viables. La recherche a consisté à développer un programme informatique permettant une simulation assistée par ordinateur. Il permet plus précisément de calculer les champs magnétiques et de concevoir les pièces du volant d'inertie afin de garantir une perte minimale d'énergie. Le champ magnétique doit être calculé en un temps raisonnable sur des distances spatiales réduites. L'approche utilisée pour répondre à ces objectifs est appliquée sur un maillage fourni par le logiciel Optiform (un remailleur adaptatif volumique développé par l'équipe GAMMA3). Les résultats obtenus ont permis d'optimiser la structure du volant d'inertie et d'atteindre une efficacité de stockage de 97%, permettant de valider la pertinence du volant et de confirmer sa fabrication.

4.13. Element metric, element quality and interpolation error metric

Participants: Paul Louis George [correspondant], Houman Borouchaki.

The metric of a simplex of $\mathbb{R}^d$ is a metric tensor (symmetric positive definite matrix) in which the element is unity (regular with unit edge lengths). This notion is related to the problem of interpolation error of a given field over a mesh. Let K be a simplex and let us denote by v_{ij} the vector joining vertex i and vertex j of K. The metric of K can be written as:

$$\mathcal{M} = \frac{d+1}{2} \Big(\sum_{i<j} v_{ij}\, {}^t v_{ij}\Big)^{-1},$$

where $v_{ij}\, {}^t v_{ij}$ is a $d \times d$ rank 1 matrix related to edge ij.

The metric of a simplex also characterizes the element shape. In particular, if it is the identity, the element is unity. Hence, to define the shape quality of an element, one can determine the gap of the element metric $\mathcal{M}$ and the identity using different measures based on the eigenvalues $\lambda_i = \frac{1}{h_I^2}$ of $\mathcal{M}$ or those of $\mathcal{M}^{-1}$, e.g. h_i^2. Notice that metric $\mathcal{M}^{-1}$ is directly related to the geometry of the element (edge length, facet area, element volume). The first algebraic shape quality measure ranging from 0 to 1 is defined as the ratio of the geometric average of the eigenvalues of $\mathcal{M}^{-1}$ and their arithmetic average:

$$q(K) = \frac{\left(\prod_i h_i^2\right)^{\frac{1}{d}}}{\frac{1}{d}\sum_{i=1}^{d} h_i^2} = d\, \frac{\left(det(\mathcal{M}^{-1})\right)^{\frac{1}{d}}}{tr(\mathcal{M}^{-1})}.$$

As the geometric average is smaller than the arithmetic average, this measure is well defined. In addition, it is the algebraic reading of the well-known quality measure defined by:

$$q^{\frac{d}{2}}(K) = (d!) d^{\frac{d}{2}} (d+1)^{\frac{d-1}{2}} \frac{|K|}{\left(\sum_{i<j} l_{ij}^2\right)^{\frac{d}{2}}},$$

where the volume and the square of the edge lengths are involved. The algebraic meaning justifies the above geometric measure. The second algebraic shape quality measure is defined as the ratio of the harmonic average of the eigenvalues of $\mathcal{M}^{-1}$ and their arithmetic average (ranging also from 0 to 1):

$$q(K) = \frac{\left\{\frac{1}{d}\sum_{i=1}^{d} \frac{1}{h_i^2}\right\}^{-1}}{\frac{1}{d}\sum_{i=1}^{d} h_i^2} = \frac{d^2}{tr(\mathcal{M})\, tr(\mathcal{M}^{-1})}.$$

As above, this measure is well defined, the harmonic average being smaller the arithmetic one. From this measure, one can derive another well-known measure involving the roundness and the size of an element (measure which is widely used for convergene issues in finite element methods).

Note that these measures use the invariants of $\mathcal{M}^{-1}$ or $\mathcal{M}$ and thus can be evaluated from the coefficients of the characteristical polynomial of those matrices (avoiding the effective calculation of their eigenvalues). Another advantage of the above algebraic shape measures is their easy extensions in an arbitrary Euclidean space. Indeed, if $\mathcal{E}$ is the metric of such a space, the algebraic shape measures read:

$$q_{\mathcal{E}}(K) = d\, \frac{\left(det(\mathcal{M}^{-1}\mathcal{E})\right)^{\frac{1}{d}}}{tr(\mathcal{M}^{-1}\mathcal{E})} \quad , \quad q_{\mathcal{E}}(K) = \frac{d^2}{tr(\mathcal{E}^{-1}\mathcal{M})\, tr(\mathcal{M}^{-1}\mathcal{E})}.$$

This work has been published in a journal, [8].

Following this notion of a element metric, a natural work was done regarding how to define the element metric so as to achieve a given accuracy for the interpolation error of a function using a finite element approximation by means of simplices of arbitrary degree.

This is a new approach for the majoration of the interpolation error of a polynomial function of arbitrary degree n interpolated by a polynomial function of degree $n-1$. From that results a metric, the so-called interpolation metric, which allows for a control of the error. The method is based on the geometric and algebraic properties of the metric of a given element, metric in which the element is regular and unit. The interpolation metric plays an important role in advanced computations based on mesh adaptation. The method relies in a Bezier reading of the functions combined with Taylor expansions. In this way, the error in a given element is fully controled at the time the edges of the element are controled.

It is shown that the error in bounded as

$$|e(X)| \leq C \sum_{i<j} f^{(n)}(.)(v_{ij}, v_{ij}, ..., v_{ij}),$$

where C is a constant depending on d and n, v_{ij} is the edge from the vertices of K of index i and j, $f^{(n)}(.)$ is the derivative of order n of f applied to a n-uple uniquely composed of v_{ij}. If we consider the case $d=2$ and $u=(x,y)$ is a vector in $\mathbb{R}^2$, we have

$$f^{(n)}(.)(u,u,...,u) = \sum_{i=0}^{n-2} x^{n-2-i} y^i \; {}^t u \left(C_i^{n-2} \mathcal{H}_{(n-2,n-2-i,i)} \right) u \;,$$

where the quadratic forms $\mathcal{H}_{(n-2,n-2-i,i)}$ are defined by the matrices of order 2 (with constant entries):

$$\mathcal{H}_{(n-2,n-2-i,i)} = \begin{pmatrix} \frac{\partial^{(n)} f}{\partial x_1^{n-i} \partial x_2^{i}} & \frac{\partial^{(n)} f}{\partial x_1^{n-1-i} \partial x_2^{i+1}} \\ \\ \frac{\partial^{(n)} f}{\partial x_1^{n-1-i} \partial x_2^{i+1}} & \frac{\partial^{(n)} f}{\partial x_1^{n-2-i} \partial x_2^{i+2}} \end{pmatrix},$$

those matrices being the hessians of the derivatives of f of order $n-2$.

This work resulted in a paper submitted in a journal and currently under revision.

4.14. Realistic modeling of fractured geologic media

Participants: Patrick Laug [correspondant], Géraldine Pichot.

This study, in collaboration with project-team Serena, aims to model, in a realistic and efficient manner, natural fractured media. These media are characterized by their diversity of structures and organizations. Numerous studies in the past decades have evidenced the existence of characteristic structures at multiple scales. At fracture scale, the aperture distribution is widely correlated and heterogeneous. At network scale, the topology is complex resulting from mutual mechanical interactions as well as from major stresses. Geometric modeling of fractured networks combines in a non-standard way a large number of 2D fractures interconnected in the 3D space. Intricate local configurations of fracture intersections require original methods of geometric modeling and mesh generation. We have developed in 2016 a software package that automatically builds geometric models and surface meshes of random fracture networks. The results are highly promising and we now want to continue this research to further improve the element quality in complex configurations, take into account multiple size scales in large fracture networks (up to thousands of fractures), and compare several modeling strategies (mixed hybrid finite elements, projected grids, mortar elements) [13].

4.15. Parallel meshing of surfaces defined by collections of connected regions

Participant: Patrick Laug [correspondant].

In CAD (computer aided design) environments, a surface is commonly modeled as a collection of connected regions represented by parametric mappings. For meshing such a composite surface, a parallelized indirect approach with dynamic load balancing can be used on a shared memory system. However, this methodology can be inefficient in practice because most existing CAD systems use memory caches that are only appropriate to a sequential process. As part of the sabbatical year of P. Laug at Polytechnique Montréal in 2014/2015, two solutions have been proposed, referred to as the Pirate approach and the Discrete approach. In the first approach, the Pirate library can be efficiently called in parallel since no caching is used for the storage or evaluation of geometric primitives. In the second approach, the CAD environment is replaced by internal procedures interpolating a discrete geometric support. In 2016, the dynamic load balancing has been analyzed and improved. Significant modifications to the Pirate library have made, and new numerical tests on three different computers (4, 8 and 64 cores) have been carried out, now showing an almost linear scaling of the method in all cases [10].

4.16. Discrete CAD model for visualization and meshing

Participants: Patrick Laug [correspondant], Houman Borouchaki.

During the design of an object using a CAD (computer aided design) platform, the user can visualize the ongoing model at every moment. Visualization is based on a discrete representation of the model that coexists with the exact analytical representation of the object. Most CAD systems have this discrete representation available, and each of them applies its own construction methodology. We have developed in 2016 a method to build a discrete model for CAD surfaces (the model is quadtree-based and subdivided into quadrilaterals and triangles). The method presents two major particularities: most elements are aligned with iso-parametric curves and the accuracy of the surface approximation is controlled. In addition, we have proposed a new technique of surface mesh generation that is based on this discrete model. This approach has been implemented as a part of a surface mesher called ALIEN, and several examples have demonstrate the robustness and computational efficiency of the program, as well as the quality of the geometric support [14], [15].

4.17. Visualization and modification of high-order curved meshes

Participants: Alexis Loyer, Dave Marcum, Adrien Loseille [correspondant].

During the partnership between Inria and Distene, a new visualization software has been designed. It address the typical operations that are required to quickly assess the newly algorithm developed in the team. In particular, interactive modifications of high-order curved mesh and hybrid meshes has been addressed. The software VIZIR is freely available at https://www.rocq.inria.fr/gamma/gamma/vizir/.

4.18. Adaptation de maillages pour des écoulements visqueux en turbomachine

Participants: Frédéric Alauzet, Loïc Frazza, Adrien Loseille [correspondant].

4.18.1. Calcul.

Les prémices d'une adaptation pour les écoulements Navier-Stokes turbulents ont été testés sur des calculs de turbomachine. Pour ce faire nous avons tout d'abord traité les particularités liées aux calculs en turbomachine: - Les aubes présentent en général une périodicité par rotation et on ne simule donc qu'une période afin d'alléger les calculs. Il faut donc traiter cette périodicité de façon appropriée dans le code CFD et l'adaptation de maillage. - Afin de prendre en compte la rotation des pales sans employer de maillages mobiles et simulations instationnaires on peut se placer dans le référentiel tournant de l'aube en corrigeant les équations. - Les écoulements en turbomachine sont des écoulements clos, les conditions limites d'entrée et de sortie ont donc une influence très forte et peuvent de plus se trouver très près de la turbine afin de simuler la présence d'autres étages en amont ou aval. Des conditions limites bien précises ont donc été développées afin de traiter correctement ces effets.

4.18.2. Adaptation.

Pour l'adaptation de maillages deux particularités doivent être traitées ici, la périodicité du maillage et la couche limite turbulente.

En 2D, la couche limite turbulente est automatiquement adaptée avec la méthode metric orthogonal et la périodicité du maillage est garantie par un traitement spécial des frontières. Les estimateurs d'erreurs Navier-Stokes et RANS n'étant pas encore au point nous avons utilisé la Hessienne du Mach de l'écoulement comme senseur ce qui donne déjà des résultats satisfaisants.

En 3D la méthode metric orthogonal est beaucoup plus complexe à mettre en oeuvre et n'est pas encore au point. La couche limite a donc été exclue de l'adaptation, le maillage est adapté uniquement dans le volume en utilisant la Hessienne du Mach de l'écoulement comme senseur. La périodicité n'étant pas traitée non plus, les frontières périodiques restent inchangées ce qui garantie leur périodicité.

4.18.3. Norm-Oriented.

Dans le cadre de la théorie Norm-Oriented, afin de contrôler l'erreur implicite des schémas numériques, un correcteur a été développé et testé. Etant donné un maillage et la solution numérique obtenue avec, le résidu de cette solution projeté sur un maillage deux fois plus fin est accumulé sur le maillage initial. Ce défaut de résidu est utilisé comme terme source dans une seconde simulation plus courte. La nouvelle solution toujours sur le meme maillage est plus proche de la solution exacte et donne une bonne estimation de l'erreur.

4.19. Metric-orthogonal and metric-aligned mesh adaptation

Participants: Frédéric Alauzet, Loïc Frazza, Adrien Loseille, Dave Marcum [correspondant].

A new algorithm to derive adaptive meshes has been introduced through new cavity-based algorithms. It allows to generate anisotropic surface and volume mesh that are aligned along the eigenvector directions. This allows us to improve the quality of the meshes and to deal naturally with boundary layer mesh generation.

Die orthogonale metric Methode erzeugt 2D-Elemente mit einem Rand, der mit der Hauptrichtung der Metrik ausgerichtet ist und einem zweiten Rand, der rechtwinklig zur ersten ist. Das erzeugende Gitter is so örtlich strukturiert wo es Anisotropie gibt. Dieses Methode wurde erfolgreich zur automatischen strukturierten Gitter Erzeugung in der turbulenten Grenzschichten für Turbomaschinen Simulationen angewendet.

4.20. Parallel mesh adaptation

Participants: Frédéric Alauzet, Adrien Loseille [correspondant].

We devise a strategy in order to generate large-size adapted anisotropic meshes $O(10^8 - 10^9)$ as required in many fields of application in scientific computing. We target moderate scale parallel computational resources as typically found in R&D units where the number of cores ranges in $O(10^2 - 10^3)$. Both distributed and shared memory architectures are handled. Our strategy is based on hierarchical domain splitting algorithm to remesh the partitions in parallel. Both the volume and the surface mesh are adapted simultaneously and the efficiency of the method is independent of the complexity of the geometry. The originality of the method relies on (i) a metric-based static load-balancing, (ii) dedicated hierarchical mesh partitioning techniques to (re)split the (complex) interfaces meshes, (iii) anisotropic Delaunay cavity to define the interface meshes, (iv) a fast, robust and generic sequential cavity-based mesh modification kernel, and (v) out-of-core storing of completing parts to reduce the memory footprint. We are able to generate (uniform, isotropic and anisotropic) meshes with more than 1 billion tetrahedra in less than 20 minutes on 120 cores [11].

4.21. Unsteady adjoint computation on dynamic meshes

Participants: Eléonore Gauci, Frédéric Alauzet [correspondant].

Adjoint formulations for unsteady problems are less common due to the extra complexity inherent in the numerical solution and storage but these methods are a great option in engineering because it takes more into account the cost function we want to minimize. Moreover the engineering applications involve moving bodies and this motion must be taken into account by the governing flow equations. We develop a model of unsteady adjoint solver on moving mesh problems. The derivation of the adjoint formulation based on the ALE form of the equations requires consideration of the dynamic meshes. Our model takes into account the DGCL.

4.22. Line solver for efficient stiff parse system resolution

Participants: Loïc Frazza, Frédéric Alauzet [correspondant].

Afin d'accélérer la résolution des problèmes raides, un line-solver á été développé. Cette méthode extrait tout d'abord des lignes dans le maillage du problème selon des critères géométriques ou physiques. Le problème peut alors être résolu exactement le long des ces lignes à moindre coût. Cette méthode est particulièrement bien adaptée aux cas où l'information se propage selon une direction privilégiée tels que les chocs, les couches limites ou les sillages. Ces cas sont généralement associés à des maillages très étirés ce qui conduit à des problèmes raides mais quasi-unidimensionnels. Ils peuvent donc être résolu efficacement par un line-solver, réduisant ainsi les temps de calculs tout en gagnant en robustesse.

4.23. Error estimate for high-order solution field

Participants: Olivier Coulaud, Adrien Loseille [correspondant].

Afin de produire des solveurs d'ordre élevé, et ainsi répondre aux exigences inhérentes à la résolution de problèmes physiques complexes, nous développons une méthode d'adaptation de maillage d'ordre élevé. Celle-ci est basée sur le contrôle par une métrique de l'erreur d'interpolation induite par le maillage du domaine. Plus précisément, pour une solution donnée, l'erreur d'interpolation d'ordre k est paramétrée par la forme différentielle $(k+1)^{\text{ième}}$ de cette solution, et le problème se réduit à trouver la plus grande ellipse incluse dans une ligne de niveau de cette différentielle. La méthode que nous avons mise au point théoriquement et numériquement est appelée "log-simplexe", et permet de produire des maillages adaptés d'ordre élevé dans un temps raisonnable, et ce en dimension 2 et 3. À l'occasion de l'International Meshing Roundtable 2016, ce travail a été présenté et publié. D'autres applications de cette méthode sont en cours d'exploitation, comme par exemple la génération de maillages adaptés courbes de surface, ou le couplage avec un solveur d'ordre élevé.

4.24. Méthode d'immersion de frontières pour la mécanique des fluides

Participants: Frédéric Alauzet [correspondant], Rémi Feuillet, Adrien Loseille.

Dans les méthodes de résolution classiques des problèmes d'interaction fluide-structure, il est usuel de représenter l'objet de manière exacte dans le maillage, c'est-à-dire avec des éléments conformes à l'objet : le maillage possède des triangles dont une arête correspond avec le bord de la géométrie immergée. Cette méthode quoique plus précise est très coûteuse en préprocessing. C'est dans ce cadre qu'est introduite la notion d'immersion de frontière (embedded geometry en anglais). Cette méthode consiste à représenter la géométrie de manière fictive. Le maillage de calcul n'est de fait plus nécessairement conforme à la géométrie de l'objet. Il s'agit donc de s'intéresser aux modifications nécessaires sur les méthodes classiques pour faire un calcul dans le cadre de l'immersion de frontières. Cela concerne les conditions aux limites et l'avancée en temps. On s'intéresse également à l'adaptation de maillage pour le cas de l'immersion. La finalité de tout ce travail est d'effectuer des calculs de coefficients aérodynamiques (portance, traînée) et de trouver des résultats du même ordre de précision que ceux en géométrie inscrite.

4.25. Optimisation de formes et CAO

Participants: Frédéric Alauzet [correspondant], Jean de Becdelièvre, Adrien Loseille.

Pour ce stage de 3 mois, l'objectif était de réaliser entièrement une optimisation aérodynamique, de la génération des modèles 3D aux calculs de la forme optimisée. Le modèle choisi était l'aile du C.R.M. (Common Research Model) de la NASA qui a été extensivement testé en soufflerie. Durand la première phase du projet, l'outils EGADS (Engineering Geometry Aircraft Design System) développé par le Aerospace Computational Design Lab (M.I.T) a été utilisé pour générer des modèles 3D paramétriques. À cette occasion, un outil facilement réutilisable de génération de modèle d'aile a été développé, ainsi que des outils de modification des modèles C.A.D. sous EGADS. Les maillages surfaciques de ces modèles ont été créés par EGADS directement et modifiés immédiatement par AMG pour les adapter au calcul. Les maillages volumiques ont, eux, été générés par GHS3D. Des calculs non visqueux sur des maillages adaptés ont alors permis d'obtenir des résultats, et de répéter l'opération jusqu'à obtenir un minimum. L'originalité de cette optimisation est que chaque calcul, à chaque itération de l'optimiseur, utilise un maillage adapté à l'aide des solutions des calculs précédents ; ce qui permet de réduire les coûts de calcul et d'augmenter la précision.

4.26. Boundary layer mesh generation

Participants: Frédéric Alauzet [correspondant], Adrien Loseille, Dave Marcum.

A closed advancing-layer method for generating high-aspect-ratio elements in the boundary layer (BL) region has been developed. This approach provides an answer to the mesh generation robustness issue as it starts from an existing valid mesh and always guarantuees a valid mesh in output. And, it handles very efficiently and naturally BL front collisions and it produces a natural smooth anisotropic blending between colliding layers. In addition, it provides a robust strategy to couple unstructured anisotropic mesh adaptation and high-aspect-ratio element pseudo-structured BL meshes. To this end, the mesh deformation is performed using the metric field associated with the given anisotropic meshes to maintain the adaptivity while inflating the BL. This approach utilizes a recently developed connectivity optimization based moving mesh strategy for deforming the volume mesh as the BL is inflated. In regards to the BL mesh generation, it features state-of-art capabilities, including, optimal normal evaluation, normal smoothing, blended BL termination, mixed-elements BL, varying growth rate, and BL imprinting on curved surfaces. Results for typical aerospace configurations are presented to assess the proposed strategy on both simple and complex geometries.

IPSO Project-Team

4. New Results

4.1. List of results

4.1.1. Landau damping in Sobolev spaces for the Vlasov-HMF model

In [25], the authors consider the Vlasov-HMF (Hamiltonian Mean-Field) model. They consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). They prove that these solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping.

4.1.2. Fast Weak-Kam Integrators for separable Hamiltonian systems

In [4], the authors consider a numerical scheme for Hamilton-Jacobi equations based on a direct discretization of the Lax-Oleinik semi-group. They prove that this method is convergent with respect to the time and space stepsizes provided the solution is Lipschitz, and give an error estimate. Moreover, They prove that the numerical scheme is a *geometric integrator* satisfying a discrete weak-KAM theorem which allows to control its long time behavior. Taking advantage of a fast algorithm for computing min–plus convolutions based on the decomposition of the function into concave and convex parts, they show that the numerical scheme can be implemented in a very efficient way.

4.1.3. The weakly nonlinear large-box limit of the 2D cubic nonlinear Schrödinger equation

In [23], the authors consider the cubic nonlinear Schrödinger (NLS) equation set on a two dimensional box of size L with periodic boundary conditions. By taking the large box limit $L \to \infty$ in the weakly nonlinear regime (characterized by smallness in the critical space), we derive a new equation set on $\mathbb{R}^2$ that approximates the dynamics of the frequency modes. This nonlinear equation turns out to be Hamiltonian and enjoys interesting symmetries, such as its invariance under Fourier transform, as well as several families of explicit solutions. A large part of this work is devoted to a rigorous approximation result that allows to project the long-time dynamics of the limit equation into that of the cubic NLS equation on a box of finite size.

4.1.4. An asymptotic preserving scheme for the relativistic Vlasov–Maxwell equations in the classical limit

In [13], the authors consider the relativistic Vlasov–Maxwell (RVM) equations in the limit when the light velocity c goes to infinity. In this regime, the RVM system converges towards the Vlasov–Poisson system and the aim of this work is to construct asymptotic preserving numerical schemes that are robust with respect to this limit. A number of numerical simulations are conducted in order to investigate the performances of our numerical scheme both in the relativistic as well as in the classical limit regime. In addition, they derive the dispersion relation of the Weibel instability for the continuous and the discretized problem.

4.1.5. Free Vibrations of Axisymmetric Shells: Parabolic and Elliptic cases

In [41], approximate eigenpairs (quasimodes) of axisymmetric thin elastic domains with laterally clamped boundary conditions (Lamé system) are determined by an asymptotic analysis as the thickness (2ε) tends to zero. The departing point is the Koiter shell model that we reduce by asymptotic analysis to a scalar model that depends on two parameters: the angular frequency k and the half-thickness ε. Optimizing k for each chosen ε, we find power laws for k in function of ε that provide the smallest eigenvalues of the scalar reductions. Corresponding eigenpairs generate quasimodes for the 3D Lamé system by means of several reconstruction operators, including boundary layer terms. Numerical experiments demonstrate that in many cases the constructed eigenpair corresponds to the first eigenpair of the Lamé system.

Geometrical conditions are necessary to this approach: The Gaussian curvature has to be nonnegative and the azimuthal curvature has to dominate the meridian curvature in any point of the midsurface. In this case, the first eigenvector admits progressively larger oscillation in the angular variable as ε tends to 0. Its angular frequency exhibits a power law relation of the form $k = \gamma\varepsilon^{-\beta}$ with $\beta = \frac{1}{4}$ in the parabolic case (cylinders and trimmed cones), and the various βs $\frac{2}{5}$, $\frac{3}{7}$, and $\frac{1}{3}$ in the elliptic case. For these cases where the mathematical analysis is applicable, numerical examples that illustrate the theoretical results are presented.

4.1.6. High frequency oscillations of first eigenmodes in axisymmetric shells as the thickness tends to zero

In [30], the lowest eigenmode of thin axisymmetric shells is investigated for two physical models (acoustics and elasticity) as the shell thickness (2ε) tends to zero. Using a novel asymptotic expansion we determine the behavior of the eigenvalue $\lambda(\varepsilon)$ and the eigenvector angular frequency $k(\varepsilon)$ for shells with Dirichlet boundary conditions along the lateral boundary, and natural boundary conditions on the other parts.

First, the scalar Laplace operator for acoustics is addressed, for which $k(\varepsilon)$ is always zero. In contrast to it, for the Lamé system of linear elasticity several different types of shells are defined, characterized by their geometry, for which $k(\varepsilon)$ tends to infinity as ε tends to zero. For two families of shells: cylinders and elliptical barrels we explicitly provide $\lambda(\varepsilon)$ and $k(\varepsilon)$ and demonstrate by numerical examples the different behavior as ε tends to zero.

4.1.7. On numerical Landau damping for splitting methods applied to the Vlasov-HMF model

In [24], we consider time discretizations of the Vlasov-HMF (Hamiltonian Mean-Field) equation based on splitting methods between the linear and non-linear parts. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that the numerical solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping. Moreover, we prove that the modified state is close to the continuous one and provide error estimates with respect to the time stepsize.

4.1.8. High-order Hamiltonian splitting for Vlasov-Poisson equations

In [5], we consider the Vlasov-Poisson equation in a Hamiltonian framework and derive new time splitting methods based on the decomposition of the Hamiltonian functional between the kinetic and electric energy. Assuming smoothness of the solutions, we study the order conditions of such methods. It appears that these conditions are of Runge-Kutta-Nyström type. In the one dimensional case, the order conditions can be further simplified, and efficient methods of order 6 with a reduced number of stages can be constructed. In the general case, high-order methods can also be constructed using explicit computations of commutators. Numerical results are performed and show the benefit of using high-order splitting schemes in that context. Complete and self-contained proofs of convergence results and rigorous error estimates are also given.

4.1.9. Uniformly accurate exponential-type integrators for Klein-Gordon equations with asymptotic convergence to classical splitting schemes in the nonlinear schrödinger limit

In [34], we introduce efficient and robust exponential-type integrators for Klein-Gordon equations which resolve the solution in the relativistic regime as well as in the highly-oscillatory non-relativistic regime without any step-size restriction under the same regularity assumptions on the initial data required for the integration of the corresponding nonlinear Schrödinger limit system. In contrast to previous works we do not employ any asymptotic or multiscale expansion of the solution. This allows us to derive uniform convergent schemes under far weaker regularity assumptions on the exact solution. In addition, the newly derived first- and second-order exponential-type integrators converge to the classical Lie, respectively, Strang splitting in the nonlinear Schrödinger limit.

4.1.10. Convergence of a normalized gradient algorithm for computing ground states

In [45], we consider the approximation of the ground state of the one-dimensional cubic nonlinear Schrödinger equation by a normalized gradient algorithm combined with linearly implicit time integrator, and finite difference space approximation. We show that this method, also called *imaginary time evolution method* in the physics literature, is locally convergent, and we provide error estimates: for an initial data in a neighborhood of the ground state, the algorithm converges exponentially towards a modified soliton that is a space discretization of the exact soliton, with error estimates depending on the discretization parameters.

4.1.11. Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations

In [8], we analyse the error behavior of operator splitting methods for highly-oscillatory differential equations. The scope of applications includes time-dependent nonlinear Schrödinger equations, where the evolution operator associated with the principal linear part is highly-oscillatory and periodic in time. In a first step, a known convergence result for the second-order Strang splitting method applied to the cubic Schrödinger equation is adapted to a wider class of nonlinearities. In a second step, the dependence of the global error on the decisive parameter $0 < \varepsilon < 1$, defining the length of the period, is examined. The main result states that, compared to established error estimates, the Strang splitting method is more accurate by a factor ε, provided that the time stepsize is chosen as an integer fraction of the period. This improved error behavior over a time interval of fixed length, which is independent of the period, is due to an averaging effect. The extension of the convergence result to higher-order splitting methods and numerical illustrations complement the investigations.

4.1.12. Solving highly-oscillatory NLS with SAM: numerical efficiency and geometric properties

In [7], we present the Stroboscopic Averaging Method (SAM), which aims at numerically solving highly-oscillatory differential equations. More specifically, we first apply SAM to the Schrödinger equation on the 1-dimensional torus and on the real line with harmonic potential, with the aim of assessing its efficiency: as compared to the well-established standard splitting schemes, the stiffer the problem is, the larger the speed-up grows (up to a factor 100 in our tests). The geometric properties of SAM are also explored: on very long time intervals, symmetric implementations of the method show a very good preservation of the mass invariant and of the energy. In a second series of experiments on 2-dimensional equations, we demonstrate the ability of SAM to capture qualitatively the long-time evolution of the solution (without spurring high oscillations).

4.1.13. Highly-oscillatory evolution equations with non-resonant frequencies: averaging and numerics

In [40], we are concerned with the application of the recently introduced multi-revolution composition methods, on the one hand, and two-scale methods, on the other hand, to a class of highly-oscillatory evolution equations with multiple frequencies. The main idea relies on a well-balanced reformulation of the problem as an equivalent mono-frequency equation which allows for the use of the two aforementioned techniques.

4.1.14. A formal series approach to the Center Manifold theorem

In [35], we consider near-equilibrium systems of ordinary differential equations with explicit separation of the slow and stable manifolds. Formal B-series like those previously used to analyze highly-oscillatory systems or to construct modified equations are employed here to construct expansions of the change of variables, the center invariant manifold and the reduced model. The new approach may be seen as a process of reduction to a normal form, with the main advantage, as compared to the standard view conveyed by the celebrated center manifold theorem, that it is possible to recover the complete solution at any time through an explicit change of variables.

4.1.15. Uniformly accurate time-splitting methods for the semi-classical Schrödinger equation, Part II: Numerical analysis

This article [39] is second part of a twofold paper devoted to the construction of numerical methods which remain insensitive to the smallness of the semiclassical parameter for the Schrödinger equation in the semiclassical limit. Here, we specifically analyse the convergence behavior of the first-order splitting introduced in Part I, for a linear equation with smooth potential. Our main result is a proof of uniform accuracy.

4.1.16. Averaging of highly-oscillatory transport equations

In [38], we develop a new strategy aimed at obtaining high-order asymptotic models for transport equations with highly-oscillatory solutions. The technique relies upon recent developments averaging theory for ordinary differential equations, in particular normal form expansions in the vanishing parameter. Noteworthy, the result we state here also allows for the complete recovery of the exact solution from the asymptotic model. This is done by solving a companion transport equation that stems naturally from the change of variables underlying high-order averaging. Eventually, we apply our technique to the Vlasov equation with external electric and magnetic fields. Both constant and non-constant magnetic fields are envisaged, and asymptotic models already documented in the literature and re-derived using our methodology. In addition, it is shown how to obtain new high-order asymptotic models.

4.1.17. Asymptotic preserving and time diminishing schemes for rarefied gas dynamic

In [11], we introduce a new class of numerical schemes for rarefied gas dynamic problems described by collisional kinetic equations. The idea consists in reformulating the problem using a micro-macro decomposition and successively in solving the microscopic part by using asymptotically stable Monte Carlo methods. We consider two types of decompositions, the first leading to the Euler system of gas dynamics while the second to the Navier-Stokes equations for the macroscopic part. In addition, the particle method which solves the microscopic part is designed in such a way that the global scheme becomes computationally less expensive as the solution approaches the equilibrium state as opposite to standard methods for kinetic equations which computational cost increases with the number of interactions. At the same time, the statistical error due to the particle part of the solution decreases as the system approach the equilibrium state. This causes the method to degenerate to the sole solution of the macroscopic hydrodynamic equations (Euler or Navier-Stokes) in the limit of infinite number of collisions. In a last part, we will show the behaviors of this new approach in comparisons to standard Monte Carlo techniques for solving the kinetic equation by testing it on different problems which typically arise in rarefied gas dynamic simulations.

4.1.18. Asymptotic Preserving scheme for a kinetic model describing incompressible fluids

The kinetic theory of fluid turbulence modeling developed by Degond and Lemou (2002) is considered for further study, analysis and simulation. Starting with the Boltzmann like equation representation for turbulence modeling, a relaxation type collision term is introduced for isotropic turbulence. In order to describe some important turbulence phenomenology, the relaxation time incorporates a dependency on the turbulent microscopic energy and this makes difficult the construction of efficient numerical methods. To investigate this problem, we focus in this work [17] on a multi-dimensional prototype model and first propose an appropriate change of frame that makes the numerical study simpler. Then, a numerical strategy to tackle the stiff relaxation source term is introduced in the spirit of Asymptotic Preserving Schemes. Numerical tests are performed in a one-dimensional framework on the basis of the developed strategy to confirm its efficiency.

4.1.19. Numerical schemes for kinetic equations in the diffusion and anomalous diffusion limits. Part I: the case of heavy-tailed equilibrium

In [15], we propose some numerical schemes for linear kinetic equations in the diffusion and anomalous diffusion limit. When the equilibrium distribution function is a Maxwellian distribution, it is well known that for an appropriate time scale, the small mean free path limit gives rise to a diffusion type equation. However, when a heavy-tailed distribution is considered, another time scale is required and the small mean free path limit leads to a fractional anomalous diffusion equation. Our aim is to develop numerical schemes for the original kinetic model which works for the different regimes, without being restricted by stability conditions of standard explicit time integrators. First, we propose some numerical schemes for the diffusion asymptotics; then, their extension to the anomalous diffusion limit is studied. In this case, it is crucial to capture the effect of the large velocities of the heavy-tailed equilibrium, so that some important transformations of the schemes derived for the diffusion asymptotics are needed. As a result, we obtain numerical schemes which enjoy the Asymptotic Preserving property in the anomalous diffusion limit, that is: they do not suffer from the restriction on the time step and they degenerate towards the fractional diffusion limit when the mean free path goes to zero. We also numerically investigate the uniform accuracy and construct a class of numerical schemes satisfying this property. Finally, the efficiency of the different numerical schemes is shown through numerical experiments.

4.1.20. Numerical schemes for kinetic equations in the anomalous diffusion limit. Part II: degenerate collision frequency

In [14], which is the continuation of [15], we propose numerical schemes for linear kinetic equation which are able to deal with the fractional diffusion limit. When the collision frequency degenerates for small velocities it is known that for an appropriate time scale, the small mean free path limit leads to an anomalous diffusion equation. From a numerical point of view, this degeneracy gives rise to an additional stiffness that must be treated in a suitable way to avoid a prohibitive computational cost. Our aim is therefore to construct a class of numerical schemes which are able to undertake these stiffness. This means that the numerical schemes are able to capture the effect of small velocities in the small mean free path limit with a fixed set of numerical parameters. Various numerical tests are performed to illustrate the efficiency of our methods in this context.

4.1.21. Multiscale schemes for the BGK-Vlasov-Poisson system in the quasi-neutral and fluid limits. Stability analysis and first order schemes

In [12], we deal with the development and the analysis of asymptotic stable and consistent schemes in the joint quasi-neutral and fluid limits for the collisional Vlasov-Poisson system. In these limits, the classical explicit schemes suffer from time step restrictions due to the small plasma period and Knudsen number. To solve this problem, we propose a new scheme stable for choices of time steps independent from the small scales dynamics and with comparable computational cost with respect to standard explicit schemes. In addition, this scheme reduces automatically to consistent discretizations of the underlying asymptotic systems. In this first work on this subject, we propose a first order in time scheme and we perform a relative linear stability analysis to deal with such problems. The framework we propose permits to extend this approach to high order schemes in the next future. We finally show the capability of the method in dealing with small scales through numerical experiments.

4.1.22. Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equations.

In [16], we deal with the numerical simulation of a Vlasov-Poisson equation modeling charged particles in a beam submitted to a highly oscillatory external electric field. A numerical scheme is constructed for this model. This scheme is uniformly accurate with respect to the size of the fast time oscillations of the solution, which means that no time step refinement is required to simulate the problem. The scheme combines the forward semi-Lagrangian method with a class of Uniformly Accurate (UA) time integrators to solve the characteristics. These UA time integrators are derived by means of a two-scale formulation of the characteristics, with the introduction of an additional periodic variable. Numerical experiments are done to show the efficiency of the proposed methods compared to conventional approaches.

4.1.23. Multi-scale methods for the solution of the radiative transfer equation

Various methods have been developed and tested over the years to solve the radiative transfer equation (RTE) with different results and trade-offs. Although the RTE is extensively used, the approximate diffusion equation is sometimes preferred, particularly in optically thick media, due to the lower computational requirements. Recently, multi-scale models, namely the domain decomposition methods, the micro-macro model and the hybrid transport- diffusion model, have been proposed as an alternative to the RTE. In domain decomposition methods, the domain is split into two subdomains, namely a mesoscopic subdomain where the RTE is solved and a macroscopic subdomain where the diffusion equation is solved. In the micro-macro and hybrid transport-diffusion models, the radiation intensity is decomposed into a macroscopic component and a mesoscopic one. In both cases, the aim is to reduce the computational requirements, while maintaining the accuracy, or to improve the accuracy for similar computational requirements. In [10], these multi-scale methods are described, and the application of the micro-macro and hybrid transport-diffusion models to a three- dimensional transient problem is reported. It is shown that when the diffusion approximation is accurate, but not over the entire domain, the multi-scale methods may improve the solution accuracy in comparison with the solution of the RTE. The order of accuracy of the numerical schemes and the radiative properties of the medium play a key role in the performance of the multi-scale methods.

4.1.24. Nonlinear Geometric Optics method based multi-scale numerical schemes for highly-oscillatory transport equations

In [42], we introduce a new numerical strategy to solve a class of oscillatory transport PDE models which is able to capture accurately the solutions without numerically resolving the high frequency oscillations in both space and time. Such PDE models arise in semiclassical modeling of quantum dynamics with band-crossings, and other highly oscillatory waves. Our first main idea is to use the nonlinear geometric optics ansatz, which builds the oscillatory phase into an independent variable. We then choose suitable initial data, based on the Chapman-Enskog expansion, for the new model. For a scalar model, we prove that so constructed model will have certain smoothness, and consequently, for a first order approximation scheme we prove uniform error estimates independent of the (possibly small) wave length. The method is extended to systems arising from a semiclassical model for surface hopping, a non-adiabatic quantum dynamic phenomenon. Numerous numerical examples demonstrate that the method has the desired properties.

4.1.25. Asymptotic Preserving numerical schemes for multiscale parabolic problems

In [18], we consider a class of multiscale parabolic problems with diffusion coefficients oscillating in space at a possibly small scale ε. Numerical homogenization methods are popular for such problems, because they capture efficiently the asymptotic behaviour as ε goes to 0, without using a dramatically fine spatial discretization at the scale of the fast oscillations. However, known such homogenization schemes are in general not accurate for both the highly oscillatory regime ($\varepsilon << 1$) and the non oscillatory regime ($\varepsilon \approx 1$). In this paper, we introduce an Asymptotic Preserving method based on an exact micro-macro decomposition of the solution which remains consistent for both regimes.

4.1.26. Uniformly accurate numerical schemes for the nonlinear dirac equation in the nonrelativistic limit regime

In [47], we apply the two-scale formulation approach to propose uniformly accurate (UA) schemes for solving the nonlinear Dirac equation in the nonrelativistic limit regime. The nonlinear Dirac equation involves two small scales ε and ε^2 with $\varepsilon \to 0$ in the nonrelativistic limit regime. The small parameter causes high oscillations in time which bring severe numerical burden for classical numerical methods. We present a suitable two-scale formulation as a general strategy to tackle a class of highly oscillatory problems involving the two small scales ε and ε^2. A numerical scheme with uniform (with respect to $\varepsilon \in [0, 1]$) second order accuracy in time and a spectral accuracy in space are proposed. Numerical experiments are done to confirm the UA property.

4.1.27. Semiclassical Sobolev constants for the electro-magnetic Robin Laplacian

In [26], we deal with the asymptotic analysis of the optimal Sobolev constants in the semiclassical limit and in any dimension. We combine semiclassical arguments and concentration-compactness estimates to tackle the case when an electromagnetic field is added as well as a smooth boundary carrying a Robin condition. As a byproduct of the semiclassical strategy, we also get exponentially weighted localization estimates of the minimizers.

4.1.28. On the MIT bag model: self-adjointness and non-relativistic limit

This paper [32] is devoted to the mathematical investigation of the MIT bag model, that is the Dirac operator on a smooth and bounded domain with certain boundary conditions. We prove that the operator is self-adjoint and, when the mass goes to infinity, we provide spectral asymptotic results.

4.1.29. Global behavior of N competing species with strong diffusion: diffusion leads to exclusion

It is known that the competitive exclusion principle holds for a large kind of models involving several species competing for a single resource in an homogeneous environment. Various works indicate that the coexistence is possible in an heterogeneous environment. We propose in [6] a spatially heterogeneous system modeling the competition of several species for a single resource. If spatial movements are fast enough, we show that our system can be well approximated by a spatially homogeneous system, called aggregated model, which can be explicitly computed. Moreover, we show that if the competitive exclusion principle holds for the aggregated model, it holds for the spatially heterogeneous model too.

4.1.30. Extended Rearrangement inequalities and applications to some quantitative stability results

In [28], we prove a new functional inequality of Hardy-Littlewood type for generalized rearrangements of functions. We then show how this inequality provides *quantitative* stability results of steady states to evolution systems that essentially preserve the rearrangements and some suitable energy functional, under minimal regularity assumptions on the perturbations. In particular, this inequality yields a *quantitative* stability result of a large class of steady state solutions to the Vlasov-Poisson systems, and more precisely we derive a quantitative control of the L^1 norm of the perturbation by the relative Hamiltonian (the energy functional) and rearrangements. A general non linear stability result has been obtained recently by Lemou, Méhats and Raphaël (2012) in the gravitational context, however the proof relied in a crucial way on compactness arguments which by construction provides no quantitative control of the perturbation. Our functional inequality is also applied to the context of 2D-Euler system and also provides quantitative stability results of a large class of steady-states to this system in a natural energy space.

4.1.31. Mate Finding, Sexual Spore Production, and the Spread of Fungal Plant Parasites

Sexual reproduction and dispersal are often coupled in organisms mixing sexual and asexual reproduction, such as fungi. The aim of this study [27] is to evaluate the impact of mate limitation on the spreading speed of fungal plant parasites. Starting from a simple model with two coupled partial differential equations, we take advantage of the fact that we are interested in the dynamics over large spatial and temporal scales to reduce the model to a single equation. We obtain a simple expression for speed of spread, accounting for both sexual and asexual reproduction. Taking Black Sigatoka disease of banana plants as a case study, the model prediction is in close agreement with the actual spreading speed (100 km per year), whereas a similar model without mate limitation predicts a wave speed one order of magnitude greater. We discuss the implications of these results to control parasites in which sexual reproduction and dispersal are intrinsically coupled.

4.1.32. Dimension reduction for rotating Bose-Einstein condensates with anisotropic confinement

In [29], we consider the three-dimensional time-dependent Gross-Pitaevskii equation arising in the description of rotating Bose-Einstein condensates and study the corresponding scaling limit of strongly anisotropic confinement potentials. The resulting effective equations in one or two spatial dimensions, respectively, are rigorously obtained as special cases of an averaged three dimensional limit model. In the particular case where the rotation axis is not parallel to the strongly confining direction the resulting limiting model(s) include a negative, and thus, purely repulsive quadratic potential, which is not present in the original equation and which can be seen as an effective centrifugal force counteracting the confinement.

4.1.33. Averaging of nonlinear Schrödinger equations with strong magnetic confinement

In [46], we consider the dynamics of nonlinear Schrödinger equations with strong constant magnetic fields. In an asymptotic scaling limit the system exhibits a purely magnetic confinement, based on the spectral properties of the Landau Hamiltonian. Using an averaging technique we derive an associated effective description via an averaged model of nonlinear Schrödinger type. In a special case this also yields a derivation of the LLL equation.

4.1.34. The Interaction Picture method for solving the generalized nonlinear Schrödinger equation in optics

The interaction picture (IP) method is a very promising alternative to Split-Step methods for solving certain type of partial differential equations such as the nonlinear Schrödinger equation used in the simulation of wave propagation in optical fibers. The method exhibits interesting convergence properties and is likely to provide more accurate numerical results than cost comparable Split-Step methods such as the Symmetric Split-Step method. In [1] we investigate in detail the numerical properties of the IP method and carry out a precise comparison between the IP method and the Symmetric Split-Step method.

4.1.35. Diffusion limit for the radiative transfer equation perturbed by a Markovian process

In [21], we study the stochastic diffusive limit of a kinetic radiative transfer equation, which is non-linear, involving a small parameter and perturbed by a smooth random term. Under an appropriate scaling for the small parameter, using a generalization of the perturbed test-functions method, we show the convergence in law to a stochastic non-linear fluid limit.

4.1.36. Estimate for P_tD for the stochastic Burgers equation

In [20], we consider the Burgers equation on $H=L^2(0,1)$ perturbed by white noise and the corresponding transition semigroup P_t. We prove a new formula for $P_tD\phi$ (where $\phi:H\to\mathbb{R}$ is bounded and Borel) which depends on ϕ but not on its derivative. Then we deduce some new consequences for the invariant measure ν of P_t as its Fomin differentiability and an integration by parts formula which generalises the classical one for gaussian measures.

4.1.37. Degenerate Parabolic Stochastic Partial Differential Equations: Quasilinear case

In [22], we study the Cauchy problem for a quasilinear degenerate parabolic stochastic partial differential equation driven by a cylindrical Wiener process. In particular, we adapt the notion of kinetic formulation and kinetic solution and develop a well-posedness theory that includes also an L^1-contraction property. In comparison to the first-order case (Debussche and Vovelle, 2010) and to the semilinear degenerate parabolic case (Hofmanová, 2013), the present result contains two new ingredients: a generalized Itô formula that permits a rigorous derivation of the kinetic formulation even in the case of weak solutions of certain nondegenerate approximations and a direct proof of strong convergence of these approximations to the desired kinetic solution of the degenerate problem.

4.1.38. An integral inequality for the invariant measure of a stochastic reaction-diffusion equation

In [19], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove an integral inequality for the invariant measure ν of a stochastic reaction-diffusion equation. Then we discuss some consequences as an integration by parts formula which extends to ν a basic identity of the Malliavin Calculus. Finally, we prove the existence of a surface measure for a ball and a half-space of H.

4.1.39. Large deviations for the two-dimensional stochastic Navier-Stokes equation with vanishing noise correlation

In [36], we are dealing with the validity of a large deviation principle for the two-dimensional Navier-Stokes equation, with periodic boundary conditions, perturbed by a Gaussian random forcing. We are here interested in the regime where both the strength of the noise and its correlation are vanishing, on a length scale ε and

$\delta(\varepsilon)$, respectively, with $0 < \varepsilon, \delta(\varepsilon) << 1$. Depending on the relationship between ε and $\delta(\varepsilon)$ we will prove the validity of the large deviation principle in different functional spaces.

4.1.40. Quasilinear generalized parabolic Anderson model

In [33], we provide a local in time well-posedness result for a quasilinear generalized parabolic Anderson model in dimension two $\partial_t u = a(u)\Delta u + g(u)\xi$. The key idea of our approach is a simple transformation of the equation which allows to treat the problem as a semilinear problem. The analysis is done within the setting of paracontrolled calculus.

4.1.41. The Schrödinger equation with spatial white noise potential

In [44], we consider the linear and nonlinear Schrödinger equation with a spatial white noise as a potential in dimension 2. We prove existence and uniqueness of solutions thanks to a change of unknown used by Hairer and Labbé (2015) and conserved quantities.

MATHERIALS Project-Team

6. New Results

6.1. Electronic structure calculations

Participants: Éric Cancès, Virginie Ehrlacher, Claude Le Bris, Antoine Levitt, Gabriel Stoltz.

In electronic structure calculation as in most of our scientific endeavors, we pursue a twofold goal: placing the models on a sound mathematical grounding, and improving the numerical approaches.

6.1.1. Molecular systems

The work of the project-team on molecular systems has focused on advanced approaches for the computation of the electronic state of molecular systems, including the effects of electronic correlation and of the environment.

In [12], E. Cancès, D. Gontier (former PhD student of the project-team, now at Université Paris Dauphine) and G. Stoltz have analyzed the GW method for finite electronic systems. This method enables the computation of excited states. To understand it, a first step is to provide a mathematical framework for the usual one-body operators that appear naturally in many-body perturbation theory. It is then possible to study the GW equations which construct an approximation of the one-body Green's function, and give a rigorous mathematical formulation of these equations. With this framework, results can be established for the well-posedness of the GW_0 equations, a specific instance of the GW model. In particular, the existence of a unique solution to these equations is proved in a perturbative regime.

Implicit solvation models aim at computing the properties of a molecule in solution (most chemical reactions indeed take place in the liquid phase) by replacing all the solvent molecules except the ones strongly interacting with the solute, by an effective continuous medium accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. In collaboration with F. Lipparini (UPMC), B. Mennucci (Department of Chemistry, University of Pisa) and J.-P. Picquemal (Paris 6), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). E. Cancès, Y. Maday, F. Lipparini and B. Stamm have also extended this approach to the more complex polarizable continuum model (PCM).

C. Le Bris has pursued his collaboration with Pierre Rouchon (Ecole des Mines de Paris) on the study of high dimensional Lindblad type equations at play in the modelling of open quantum systems. In order to complement and better understand the numerical approaches developed in the past couple of years, some theoretical aspects are now under study, in particular regarding the well-posedness of the equations and their convergence in the long time limit.

6.1.2. Crystals and solids

Periodic systems are mathematically treated using Bloch theory, raising specific theoretical and numerical issues.

A. Bakhta (CERMICS) and V. Ehrlacher are working on the design of an efficient numerical method to solve the inverse band structure problem. The aim of this work is the following: given a set of electronic bands partially characterizing the electronic structure of a crystal, is it possible to recover the structure of a material which could achieve similar electronic properties? The main difficulty in this problem relies in the practical resolution of an associated optimization problem with numerous local optima.

As an external collaborator of the MURI project on 2D materials (PI: M. Luskin), E. Cancès has started a collaboration with P. Cazeaux and M. Luskin (University of Minnesota) on the computation of the electronic and optical properties of multilayer 2D materials. Together with E. Kaxiras (Harvard) and members of his group, they have developped a perturbation method for computing the Kohn-Sham density of states of incommensurate bilayer systems. They have also adapted the C*-algebra framework for aperiodic solids introduced by J. Bellissard and collaborators, to the case of tight-binding models of incommensurate (and possibly disordered) multilayer systems [36].

É. Cancès, A. Levitt and G. Stoltz, in collaboration with G. Panati (Rome) have proposed a new method for the computation of Wannier functions, a standard post-processing of density functional theory computations [38]. Compared to previous approaches, it does not require an initial guess for the shape of the Wannier functions, and is therefore more robust.

6.1.3. Numerical analysis

Members of the project-team have worked on the numerical analysis of partial differential equations arising from electronic structure theory.

E. Cancès and N. Mourad (CERMICS) have clarified the mathematical framework underlying the construction of norm-conserving semilocal pseudopotentials for Kohn-Sham models, and have proved the existence of optimal pseudopotentials for a family of optimality criteria.

E. Cancès has pursued his long-term collaboration with Y. Maday (UPMC) on the numerical analysis of electronic structure models. Together with G. Dusson (UMPC), B. Stamm (UMPC), and M. Vohralík (Inria), they have designed a new post processing method for planewave discretizations of nonlinear Schrödinger equations, and used it to compute sharp *a posteriori* error estimators for both the discretization error and the algorithmic error (convergence threshold in the iterations on the nonlinearity). They have then extended this approach to the Kohn-Sham model. In parallel, they have derived a posteriori error estimates for conforming numerical approximations of the Laplace eigenvalue problem with homogeneous Dirichlet boundary conditions [37]. In particular, upper and lower bounds for any simple eigenvalue are established. These bounds are guaranteed, fully computable, and converge with the optimal rate to the exact eigenvalue.

A. Levitt, in collaboration with X. Antoine and Q. Tang (Nancy), has proposed a new numerical method to compute the ground state of rotating Bose-Einstein condensates [31]. This method combines a nonlinear conjugate gradient method with efficient preconditionners. Compared to the state of the art (implicit timestepping on the imaginary-time equation), gains of one to two orders of magnitude are achieved.

6.2. Complex fluids

Participant: Sébastien Boyaval.

The aim of the research performed in the project-team about complex fluids is to guide the mathematical modelling of gravity flows with a free-surface for application to the hydraulic engineering context, and to account for non-Newtonian rheologies in particular (like in mudflows for instance). On the one hand, thin-layer (reduced) models have long been favored, and one current trend aims at incorporating non-Newtonian effects [10]. This has stimulated some research about a new hyperbolic PDE system [35]. On the other hand, there is currently a strong need to perform full 3D numerical simulations using new non-Newtonian models in complex geometries with a view to comparing them with physical observations ; this is an ongoing work, in the framework of the ANR project SEDIFLO with E. Audusse (Paris 13), A. Caboussat (Genève), A. Lemaitre (ENPC), M.Parisot (Inria).

6.3. Homogenization

Participants: Michaël Bertin, Ludovic Chamoin, Virginie Ehrlacher, Thomas Hudson, Marc Josien, Claude Le Bris, Frédéric Legoll, François Madiot, Pierre-Loïk Rothé.

6.3.1. Deterministic non-periodic systems

The homogenization of (deterministic) non-periodic systems is a well-known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc (Paris 7) and P.-L. Lions (Collège de France), C. Le Bris has introduced a possible theory, giving rise to a numerical approach, for the simulation of multiscale non-periodic systems. In former publications, several theoretical aspects have been considered, for the case of linear elliptic equations in divergence form. In the context of the PhD thesis of M. Josien, new issues are being explored, including the rate of convergence of the approximation, along with the convergence of the Green functions associated to the problems under consideration. The studies are motivated by several practically relevant problems, in particular the problem of defects in periodic structures and the "twin boundaries" problem in materials science. Also, some other equations than linear elliptic equations in divergence form have been considered lately. The case of advection-diffusion equations is currently examined. In addition, one ongoing work, in collaboration with P. Souganidis (University of Chicago) and P. Cardaliaguet (Université Paris-Dauphine), considers the non-periodic setting for Hamilton-Jacobi type equations.

6.3.2. Stochastic homogenization

The project-team has pursued its efforts in the field of stochastic homogenization of elliptic equations, aiming at designing numerical approaches that both are practically relevant and keep the computational workload limited.

Using standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the whole space $\mathbb{R}^d$. This equation is therefore delicate and expensive to solve. In practice, the space $\mathbb{R}^d$ is truncated to some bounded domain, on which the corrector problem is numerically solved. In turn, this yields a converging approximation of the homogenized tensor, which happens to be a random matrix.

Over the past years, the project-team has proposed several variance reduction techniques, which have been reviewed and compared to one another in [9], [20]. In particular, in [23], C. Le Bris, F. Legoll and W. Minvielle have investigated the possibility to use a variance reduction technique based on computing the corrector equation only for selected environments. These environments are chosen based on the fact that their statistics in the finite supercell matches the statistics of the materials in the infinite supercell. The efficiency of the approach has been demonstrated for various types of random materials, including composite materials with randomly located inclusions.

Besides the (averaged) behavior of the oscillatory solution u_ε on large space scales (which is given by the homogenized limit u_* of u_ε), another question of interest is to understand how much u_ε fluctuates around its coarse approximation u_*. This question will be explored in the PhD thesis of P.-L. Rothé, which started in October 2016.

Still another question investigated in the project-team is to find an alternative to standard homogenization techniques when the latter are difficult to use in practice, because not all the information on the microscopic medium is available. Following an interaction with A. Cohen (Paris 6), C. Le Bris, F. Legoll and S. Lemaire (post-doc in the project-team until 2015), have shown that the constant matrix that “best” (in a sense made precise in [44]) represents the oscillatory matrix describing the medium converges to the homogenized matrix in the limit of infinitely rapidly oscillatory coefficients. Furthermore, the corresponding optimization problem can be efficiently solved using standard algorithms and yield accurate approximation of the homogenized matrix. It has also been shown that it is possible to construct, in a second stage, approximations to the correctors, in order to recover an approximation of the *gradient* of the solution. The details are now available in [44].

6.3.3. Multiscale Finite Element approaches

From a numerical perspective, the Multiscale Finite Element Method (MsFEM) is a classical strategy to address the situation when the homogenized problem is not known (e.g. in difficult nonlinear cases), or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as a sufficiently accurate approximation).

The MsFEM has been introduced almost 20 years ago. However, even in simple deterministic cases, there are still some open questions, for instance concerning multiscale advection-diffusion equations. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interplays with the multiscale character of the equation is an unsolved mathematical question worth considering for numerical purposes.

In the context of the PhD thesis of F. Madiot, current efforts are focused on the study of an advection-diffusion equation with a dominating convection in a perforated domain. The multiscale character of the problem stems here from the geometry of the domain. On the boundary of the perforations, we set either homogeneous Dirichlet or homogeneous Neumann conditions. In the spirit of the work [21], the purpose of our ongoing work is to investigate, on perforated domains, the behavior of several variants of the Multiscale Finite Element method, specifically designed to address multiscale advection-diffusion problems in the convection-dominated regime. Generally speaking, the idea of the MsFEM is to perform a Galerkin approximation of the problem using specific basis functions that are precomputed (in an offline stage) and adapted to the problem considered. All the variants considered are based upon local functions satisfying weak continuity conditions in the Crouzeix-Raviart sense on the boundary of mesh elements. Several possibilities for the basis functions have been examined (for instance, they may or may not encode the convection field). Depending on how basis functions are defined, stabilization techniques (such as SUPG) may be required. The type of boundary conditions on the perforations (either homogeneous Dirichlet or homogeneous Neumann boundary conditions) drastically affects the nature of the flow, and therefore the conclusions regarding which numerical approach is best to adopt. In short, homogeneous Dirichlet boundary conditions on the perforations damp the effect of advection, making the flow more stable than it would be in the absence of perforations, while this is not the case for homogeneous Neumann boundary conditions. This intuitive fact is investigated thoroughly at the numerical level, and particularly well exemplified, at the theoretical level, by the comparison of the respective homogenization limits.

Advection-diffusion equations that are both non-coercive and advection-dominated have also been considered (in a single-scale framework). Many numerical approaches have been proposed in the literature to address such difficult cases. C. Le Bris, F. Legoll and F. Madiot have proposed an approach based on the invariant measure associated to the original equation. The approach has been summarized in [22], and extensively described, analyzed and numerically tested in [45]. It is shown there that this approach allows for an unconditionally well-posed finite element approximation, and that it can be stable, as accurate as, and more robust than classical stabilization approaches.

Most of the numerical analysis studies of the MsFEM are focused on obtaining *a priori* error bounds. In collaboration with L. Chamoin, who was on leave in the project-team (from ENS Cachan, from September 2014 to August 2016), members of the project-team have been working on *a posteriori* error analysis for MsFEM approaches, with the aim of developing error estimation and adaptation tools. They have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution u_h has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux $k\nabla u$. In the context of the MsFEM, it is important to be able to perform all expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach thus needs to be adapted to that context. The proposed approach yields very interesting results, and provides an accurate and robust estimation of the global error. The approach has also been adapted towards the design of adaptive algorithms for specific quantities of interest (in the so-called "goal-oriented" setting), and towards the design of model reduction approaches (such as the Proper Generalized Decomposition (PGD)) in the specific context of multiscale problems. The work will be reported on in a forthcoming publication in preparation.

6.3.4. Discrete systems and their thermodynamic limit

In collaboration with X. Blanc (Paris 7), M. Josien has studied the macroscopic limit of a chain of atoms governed by Newton's equations. It is known from the works of X. Blanc (Paris 7), C. Le Bris and P.-L. Lions (Collège de France) that this limit is the solution of a nonlinear wave equation, as long as the solution remains smooth. For a large class of interaction potentials, X. Blanc and M. Josien have shown in [34], theoretically and numerically, that, if the distance between particles remains bounded, the above description in terms of a non-linear wave equation equation no longer holds when there are shocks. Indeed, the system of particles produces dispersive waves that are not predicted by the nonlinear wave equation.

6.3.5. Dislocations

Plastic properties of crystals are due to dislocations, which are thus objects of paramount importance in materials science. The geometrical shape of dislocations may be described by (possibly time-dependent) nonlinear integro-differential equations (e.g. Weertman's equation and the dynamical Peierls-Nabarro equation), involving non-local operators. In collaboration with Y.-P. Pellegrini (CEA), M. Josien has first focused on the steady state regime (where the equation of interest is the Weertman equation), and has designed an efficient numerical method for approximating its solution. The approach is based on a splitting strategy between the nonlinear local terms (which are integrated in real space) and the linear nonlocal terms (which are integrated in Fourier space). Current efforts are devoted to the simulation of physically relevant test-cases, with the aim of comparing the obtained numerical results with results of the physics literature. The work will be reported on in a forthcoming publication in preparation.

6.4. Computational Statistical Physics

Participants: Grégoire Ferré, Giacomo Di Gesù, Thomas Hudson, Dorian Le Peutrec, Frédéric Legoll, Tony Lelièvre, Pierre Monmarché, Boris Nectoux, Julien Roussel, Mathias Rousset, Laura Silva Lopes, Gabriel Stoltz, Pierre Terrier, Pierre-André Zitt.

In [24], T. Lelièvre and G. Stoltz have given an overview of state-of-the art mathematical techniques which are useful to analyze and quantify the efficiency of the algorithms used in molecular dynamics, both for sampling thermodynamic quantities (canonical averages and free energies) and dynamical quantities (transition rates, reactive paths and transport coefficients).

6.4.1. Improved sampling methods

This section is devoted to recent methods which have been proposed in order to improve the sampling of the canonical distribution by modifying the Langevin or overdamped Langevin dynamics, or its discretization. Two general strategies have been pursued by the project-team along these lines: (i) constructing dynamics with better convergence rate and hence smaller statistical errors; (ii) the stabilization of discretization schemes by Metropolis procedures in order to allow for larger timesteps while maintaining acceptable rejection rates.

A first approach to obtaining better convergence rates consists in modifying the drift term in the overdamped-Langevin dynamics, in order to improve the rate of converge to equilibrium. This method was considered by T. Lelièvre with A. Duncan and G.A. Pavliotis (Imperial College) in [14]. It is shown that nonreversible dynamics always result in a smaller asymptotic variance (statistical error). The efficiency of the whole algorithm crucially depends on the time discretization, which may induce some bias (deterministic error). It is shown on some examples how to balance the two errors (bias and statistical errors) in order to obtain an efficient algorithm.

The discretization of overdamped Langevin dynamics, using schemes such as the Euler-Maruyama method, may lead to numerical methods that are unstable when the forces are non-globally Lipschitz. One way to stabilize numerical schemes is to superimpose some acceptance/rejection rule, based on a Metropolis-Hastings criterion for instance. However, rejections perturb the dynamical consistency of the resulting numerical method with the reference dynamics. G. Stoltz and M. Fathi (Toulouse) present in [15] some modifications of the standard stabilization of discretizations of overdamped Langevin dynamics by a Metropolis-Hastings procedure, which allow to either improve the strong order of the numerical method, or to reduce the bias in the estimation of transport coefficients characterizing the effective dynamical behavior of the dynamics.

The sampling properties of Langevin dynamics can be improved by considering more general non-quadratic kinetic energies. This was accomplished in [26], where G. Stoltz, with S. Redon and Z. Trstanova (Inria Grenoble), have studied the properties of Langevin dynamics with general, non-quadratic kinetic energies $U(p)$, showing in particular the ergodicity of the dynamics even when the kinetic force ∇U vanishes on open sets and proving linear response results for the variance of the process for kinetic energies which correspond to the so-called adaptively restrained particle simulations. This work has been complemented by [51], where G. Stoltz and Z. Trstanova provide accurate numerical schemes to integrate the modified Langevin dynamics with general kinetic energies, with possibly non globally Lipschitz momenta.

6.4.2. Adaptive methods

When direct sampling methods fail, it is worth considering importance sampling strategies, where the slowest direction is described by a reaction coordinate ξ, and the invariant measure is biased by (a fraction of) the free energy associated with ξ.

The first group of results along these lines concerns the study of adaptive biasing methods to compute free energy differences:

- The result obtained by H. Al Rachid (CERMICS) in collaboration with T. Lelièvre and R. Talhouk (Beirut) on the existence of a solution to the non linear Fokker Planck equation associated to the ABF process has been published, see [7].
- T. Lelièvre and G. Stoltz, together with G. Fort (Toulouse) and B. Jourdain (CERMICS), have studied the well-tempered metadynamics and many variants of this method in [41]. This dynamics can be seen as some extension of the so-called self-healing umbrella sampling method, with a partial biasing of the dynamics only. In particular, the authors propose a version which leads to much shorter exit times from metastable states (accelerated well-tempered metadynamics).

The project-team also works on adaptive splitting techniques, which forces the exploration in the direction of increasing values of the reaction coordinate. In [29], T. Lelièvre, together with C. Mayne, K. Schulten and I. Teo (Univ. Illinois), has reported on the calculation of the unbinding rate of the benzamidine-trypsin system using the Adaptive Multilevel Splitting algorithm. This is the first "real-life" test case for the adaptive multilevel splitting. In [11], T. Lelièvre and M. Rousset, in collaboration with C.E. Bréhier (Lyon), M. Gazeau (Créteil) and L. Goudenège (Centrale), propose a generalization of the Adaptive Multilevel Splitting method for discrete-in-time processes. It is shown how to make the estimator unbiased. Numerical experiments illustrate the performance of the method.

6.4.3. Coarse-graining and reduced descriptions

A fully atomistic description of physical systems leads to problems with a very large of unknowns, which raises challenges both on the simulation of the system and the interpretation of the results. Coarse-grained approaches, where complex molecular systems are described by a simplified model, offer an appealing alternative.

F. Legoll and T. Lelièvre, together with S. Olla (Dauphine), have proposed an analysis of the error introduced when deriving an effective dynamics for a stochastic process in large dimension on a few degrees of freedom using a projection approach à la Zwanzig [48]. More precisely, a pathwise error estimate is obtained, which is an improvement compared to a previous result by F. Legoll and T. Lelièvre where only the marginal in times were considered.

Another line of research concerns dissipative particle dynamics, where a complex molecule is replaced by an effective mesoparticle. The work [17] by G. Stoltz, together with A.-A. Homman and J.-B. Maillet (CEA), on new parallelizable numerical schemes for the integration of Dissipative Particle Dynamics with Energy conservation, has been published. Together with G. Faure and J.-B. Maillet, G. Stoltz has proposed in [16] a new formulation of smoothed dissipative particle dynamics, which can be seen as some meshless discretization of the Navier–Stokes equation perturbed by some random forcing arising from finite size effects of the underlying mesoparticles. The reformulation, in terms of internal energies rather than internal entropies, allows for a simpler and more efficient simulation, and also opens the way for a coupling with standard dissipative particle dynamics models.

G. Stoltz also suggested in [50] a new numerical integrator for DPDE which is more stable than all the previous integrators. The key point is to reduce the stochastic part of the dynamics to elementary one-dimensional dynamics, for which some Metropolis procedure can be used to prevent the appearance of negative energies at the origin of the instability of the numerical methods.

During the post-doctoral stay of I.G. Tejada (ENPC), G. Stoltz, F. Legoll and E. Cancès studied in collaboration with L. Brochard (ENPC) the derivation of a concurrent coupling technique to model fractures at the atomistic level by combining a reactive potential with a reduced harmonic approximation. The results have appeared in [28].

G. Stoltz and P. Terrier, in a joint work with M. Athènes, T. Jourdan (CEA) and G. Adjanor (EDF), have presented a coupling algorithm for cluster dynamics [52]. Rate equation cluster dynamics (RECD) is a mean field technique where only defect concentrations are considered. It consists in solving a large set of ODEs (one equation per cluster type) governing the evolution of the concentrations. Since clusters might contain up to million of atoms or defects, the number of equations becomes very large. Therefore solving such a system of ODEs becomes computationally prohibitive as the cluster sizes increase. Efficient deterministic simulations propose an approximation of the equations for large clusters by a single Fokker-Planck equation. The proposed coupling algorithm is based on a splitting of the dynamics and combines deterministic and stochastic approaches. In addition, F. Legoll and G. Stoltz have proposed in [19], with T. Jourdan (CEA) and L. Monasse (CERMICS), a new method for numerically integrating the Fokker–Planck approximation of large cluster dynamics.

6.4.4. Eyring–Kramers formula and quasi-stationary distributions

G. Di Gesù, T. Lelièvre and B. Nectoux, together with D. Le Peutrec, have explored the interest of using the quasi-stationary distribution approach in order to justify kinetic Monte Carlo models, and more precisely their parameterizations using the Eyring-Kramers formulas, which provide a simple rule to compute transition rates from one state to another [13]. The paper is essentially a summary of the results which have been obtained during the first two years of the PhD of B. Nectoux. A preprint with detailed proofs of these results is in preparation.

In [33], G. Di Gesù has studied with N. Berglund (Orléans) and H. Weber (Warwick) the spectral Galerkin approximations of an Allen-Cahn equation over the two-dimensional torus perturbed by weak space-time white noise. They show sharp upper and lower bounds on the transition times from a neighborhood of the stable configuration -1 to the stable configuration 1 in the small noise regime. These estimates are uniform in the discretization parameter, suggesting an Eyring-Kramers formula for the limiting renormalized stochastic PDE.

6.4.5. Functional inequalities and theoretical aspects

The interplay between probability theory and analysis in statistical physics is best exemplified by the functional analysis study of the semigroups associated with the generator of the stochastic processes under consideration. These generators are elliptic or hyperbolic operators. Several functional-analytic results were obtained by the team on problems of statistical physics.

D. Le Peutrec has derived Brascamp-Lieb type inequalities for general differential forms on compact Riemannian manifolds with boundary from the supersymmetry of the semiclassical Witten Laplacian [47]. These results imply the usual Brascamp-Lieb inequality and its generalization to compact Riemannian manifolds without boundary.

T. Hudson has considered with C. Hall (Oxford) and P. van Meurs (Univ. Kanazawa, Japan) the minimization of the potential energy of N particles mutually interacting under a repulsive interaction potential with a certain algebraic decay assumption [42]. A major novelty of the approach is that it does not assume a finite range of interaction. The main focus of the work is on characterizing the boundary behavior of minimizers in the limit where the number of particles N tends to infinity with a constant density of particles per unit volume.

G. Di Gesù has studied with M. Mariani (Rome) the small temperature limit of the Fisher information of a given probability measure with respect to the canonical measure with density proportional to $\exp(-\beta V)$ [39]. The expansion reveals a hierarchy of multiple scales reflecting the metastable behavior of the underlying overdamped Langevin dynamics: distinct scales emerge and become relevant depending on whether one considers probability measures concentrated on local minima of V, probability measures concentrated on critical points of V, or generic probability measures on $\mathbb{R}^d$.

6.5. Various topics

Participants: Virginie Ehrlacher, Tony Lelièvre, Antoine Levitt.

In [18], T. Lelièvre has explored with J. Infante Acevedo (CERMICS) the interest of using the greedy algorithm (also known as the Proper Generalized Decomposition) for the pricing of basket options.

V. Ehrlacher and D. Lombardi have developped a new tensor-based numerical method for the resolution of kinetic equations [40] in a fully Eulerian framework.This theory enables to describe a large system of particles by a distribution function $f(x,v,t)$ that encodes the probability of finding a particle at time t, position $x \in \mathbb{R}^3$ and velocity $v \in \mathbb{R}^3$. These systems are used to model the behavior of plasma of the transport of electrons in semiconductors for instance. However, simulating such systems involves the resolutions of problems defined on $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+$, which leads to very high-dimensional systems. The new approach developped in [40] circumvents the curse of dimensionality for these systems, by efficiently adapting the rank of the decomposition of the solution through time. Encouraging preliminary numerical results have been obtained on $3D \times 3D$ systems.

A system of cross-diffusion equations has been proposed in [32] by A. Bakhta and V. Ehrlacher for the modelling of a Physical Vapor Deposition (PVD) process used for the manufacturing of thin film solar cells. This process works as follows: a substrate wafer is introduced in a hot chamber where different chemical species are injected under gaseous form. These different species deposit on the surface of the substrate, so that a thin film layer grows upon the surface of the substrate. Two phenomena have to be taken into account in the modelling: 1) the evolution of the thickness of the thin film layer; 2) the diffusion of the various species inside the bulk. The existence of a weak solution to the system proposed in [32] has been proved, along with the existence of optimal fluxes to be injected in the chamber in order to obtain target concentration profiles at the end of the process. The long-time behavior of solutions has been studied in the case when the injected fluxes are constant. Moreover, numerical results on the simulation of this system have been compared with experimental data given by IRDEP on CIGS (Copper, Indium, Gallium, Selenium) solar cells. The project is a collaboration with IRDEP.

A. Levitt, in collaboration with F. Aviat, L. Lagardère, Y. Maday, J.-P. Piquemal (UPMC), B. Stamm (Aachen), P. Ren (Texas) and J. Ponder (Saint Louis), has proposed a new method for the solution of the equations of polarizable force fields [8]. Previous methods had to solve a linear system to high accuracy in order for the energy to be preserved in simulations. The method presented, based on an explicit differentiation of the energy produced by the truncated iterative method, is able to conserve the energy even with loose convergence criteria, thus allowing stable and fast simulations at degraded accuracy.

MEMPHIS Project-Team

7. New Results

7.1. Hybrid POD/DNS: application to aeroelastic windturbine blade

Some new techniques related to Reduced Order Modelling have been developed in the framework of the EU project AEROGUST. The first proposed approach is based on a domain decomposition method in which a POD [56], [43], [44], [37], [36] model is dynamically coupled with a CFD solver [39], [38]. This tool can be used to perform predictive simulations thanks to the fact that the non-linear effects related to new working conditions are directly captured by the CFD solver while the far field region can be efficiently described by the POD model. The hybrid technique has been extended to gust simulations by the introduction of forcing terms which can describe perturbations coming from the far field.
The domain decomposition approach has been proposed also inside an iterative procedure named "numerical zoom" which is based on the use of several mesh levels. This procedure is repeated several times in order to focus the degrees of freedom of the discretisation in the region close to the body.
Finally, the POD method has been proposed also for the acceleration of CFD solver for incompressible flows. The solution of the Poisson problem on the pressure variable which appears in incompressible solvers can be quite time consuming. The proposed approach consists in searching the solution of the Poisson problem in the space spanned by the POD basis. This is done by substituting the POD expansion in the Poisson equation and minimizing the residuals. The robustness of the method has been improved by introducing a check on the quality of the Poisson solution (based on the divergence of the velocity field at the end of the correction step) and a dynamic update of the POD basis.
The domain decomposition approach with the forcing terms has been used to simulate the effects of a gust on a wind turbine blade in a simplified configuration at low Reynolds number. The numerical zoom procedure is applied by coupling a DNS simulation with a POD description of the far field. The solution obtained on three levels of mesh is reported in Figure 9 in which the vortex structures are shown according to the q-criterion. The bending of the blade is described by a non-linear beam model. Figure 10 shows the shapes of the blade without loads, in the chosen working condition and during the gust.

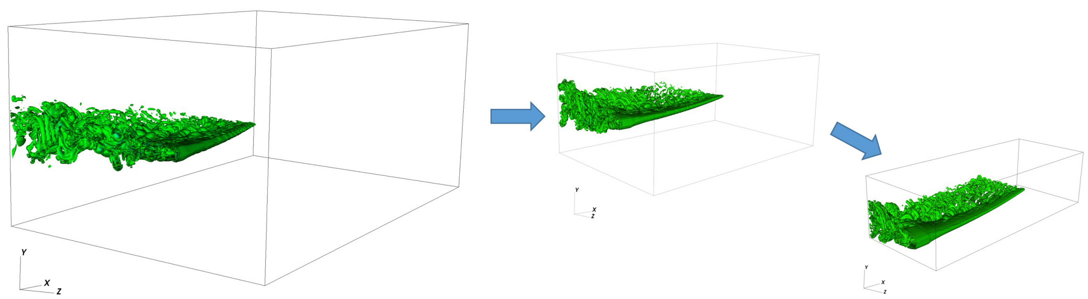
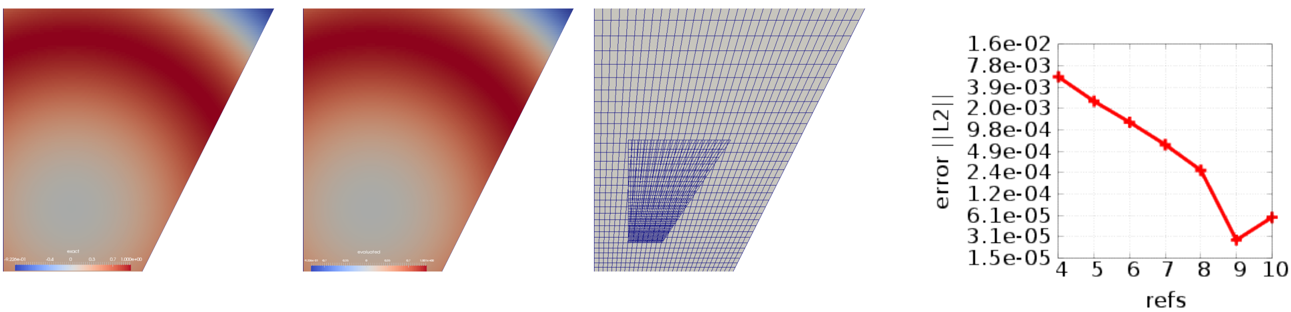


Figure 9. Numerical zoom on the wind turbine blade simulation (vortex structure visualised by q-criterion)

Figure 10. Blade shape without loads (top), in the chosen working condition (middle) and during the gust (bottom)

7.2. Discretization of the Laplacian operator using a multitude of overlapping cartesian grids

A new finite-difference approach to solve a Laplacian operator has been developed, using patches of overlapping grids where a fined level is needed, leaving coarser meshes in the rest of the computational domain. These overlapping grids will have generic quadrilateral shapes (as shown in figure 11).



(a) Exact: $sin((x-0.5)^2+(y-0.5)^2)$ (b) Evaluated (c) Numerical grid (d) Numerical error

Figure 11. results

A monolithic approach is used to solve the algebraic equations, applying restriction and prolongation operators to fill the non-diagonal blocks of the resulting matrix. These operators works on data structures communicated between the different grids using ad hoc parallel inter-communicators, as shown in figure 12 . 12 .

Works are going on to change the solver from the finite-difference approach to a finite-volume one, and to implement the 3D case. The use of a finite-volume solver can benefit from the usage of octree patches instead of cartesian grids, obtaining a more accurate refining and a greater precision.

7.3. Numerical simulation of a biomimetic LVAD developed by CorWave

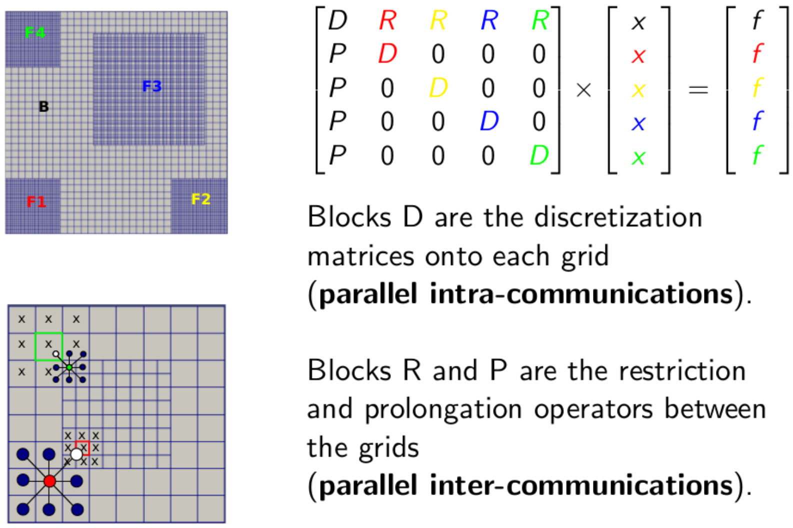


Figure 12. Monolithic approach

We just started a collaboration with the PME CorWave. The CorWave LVAD utilizes an undulating disc wave pumping mechanism, replacing the high speed, high shear impeller of current continuous flow rotary pumps. Louis de Lillers, the CorWave project manager, has contacted MEMPHIS to perform numerical simulations and optimizations of their LVAD. This collaboration has started with an industrial PhD (Cifre, Antoine Fondaneche). Figure 13 shows preliminary results (proof of concept) for the CorWave LVAD obtained with the code NaSCar described in [38].

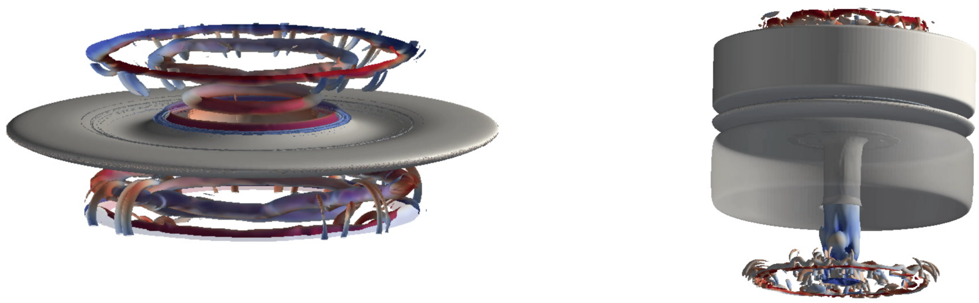


Figure 13. Preliminary results (proof of concept) for the CorWave LVAD. Left: oscillating membrane, right: the whole pump system.

7.4. A sharp Cartesian method for incompressible flows with large density ratios

We have developed and validated a new Cartesian method for bifluid incompressible flows with high density ratios. The specificity of the method relies on a sharp second order numerical scheme for the spatial resolution of the discontinuous elliptic problem for the pressure, that was developed in [42]. The Navier-Stokes equations are integrated in time thanks to a fractional step method based on the Chorin scheme and discretized in space on a Cartesian mesh. The bifluid interface is implicitly represented using a level set function. The numerical tests show the improvements due to this sharp method compared to classical first order methods. As an illustration, we present here numerical results for the dam break test case.

This test case is studied in [53] and [41], and based on experiments conducted in [49]. The initial configuration is a water column at rest in air. The initial height and width of the column are both 5.715 cm. The domain size is 40 cm×10 cm. The value of the physical parameters are

$$\begin{cases} \rho_{water} = 1000 \ kg/m^3, \\ \mu_{water} = 1.137 \times 10^{-3} \ kg/ms, \\ \rho_{air} = 1.226 \ kg/m^3, \\ \mu_{air} = 1.78 \times 10^{-5} \ kg/ms, \\ \sigma = 0.0728 \ kg/s^2 \\ g = -9.8 m/s^2 \end{cases} \tag{1}$$

We present in Figure 14 the interface evolution at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$, with h the initial height of the water column. The computations are performed with 256×64 points.

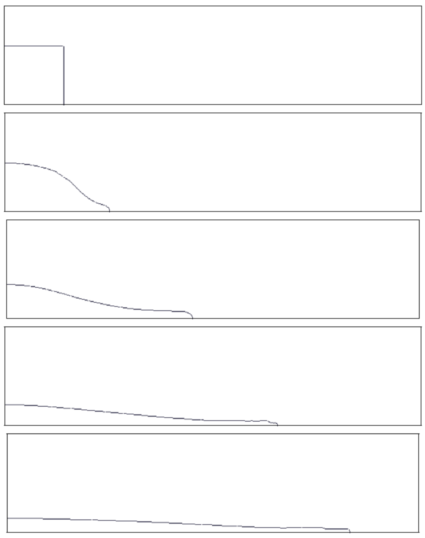


Figure 14. Evolution of the interface for the dam break problem at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$.

In Figure 15 , we plot the evolution in time of the water front, compared to the experimental results of [49], and to the results obtained for the Ghost-Fluid method and the conservative method of Raessi and Pitsch [53]. We observe that the front propagation is in agreement with the experimental results and the results of the conservative method presented in [53]. It means that, though the method is not strictly conservative, the numerical errors due to momentum transfer across the interface are not large enough to slow down the propagation of the front. It is not the case for instance for the Ghost-Fluid method, as it can be noticed in Figure 15 and has been reported in [53].

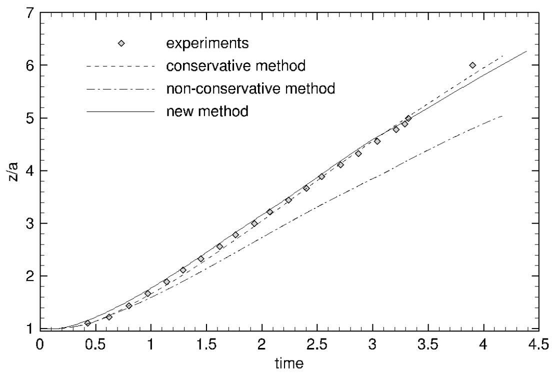


Figure 15. Evolution of the front of propagation: comparison between experimental date and several numerical methods: the Ghost Fluid method (non-conservative method), the conservative method of Raessi and Pitsch and our new method, The dimensionless location of the front $\frac{z}{a}$ is plotted as a function of the dimensionless time $t\sqrt{q}h$.

7.5. Platooning of trucks on highways

In the context of energy saving, the platooning of ground vehicles on top of a road, in particular highways has been studied. The numerical simulations are performed in 2D and 3D for up to 10 billions unknowns on 384 cores. The goal is to have trucks autonomously following their leader to form a road train in order to improve traffic flow efficiency and to reduce oil consumption. Thus the distance between trucks is short. For instance a gain of about 40% can be obtained on the drag coefficient of the followers when the distance between trucks is equal to 1.8125 their height (see the figure 16), that is approximately eight meters. Even the leader has a lower drag coefficient (-10%) as the first follower compresses the flow in its wake. In the figure it is clearly shown that the pressure gradients inside the gap between the vehicles are much lower than in front of the leader.

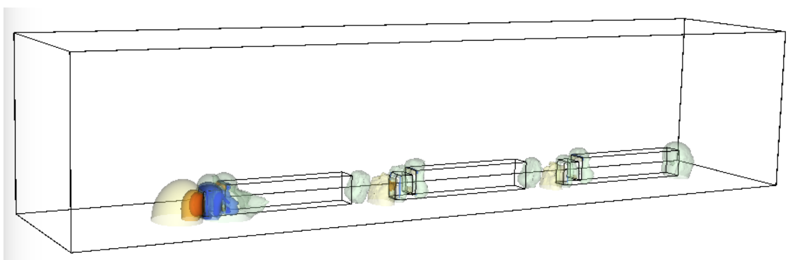


Figure 16. Mean pressure contours of the mean flow around three simplified European tractor-trailer geometries with a distance equal to 1.8125 their height on top of a road in three dimensions.

7.6. Non-linear elasto-plastic dynamics of compressible materials

We describe a numerical model to simulate the non-linear elasto-plastic dynamics of compressible materials. The model is fully Eulerian and it is discretized on a fixed Cartesian mesh. The hyperelastic constitutive law considered is neohookean and the plasticity model is based on a multiplicative decomposition of the inverse deformation tensor. The model is thermodynamically consistent and it is shown to be stable in the sense that the norm of the deviatoric stress tensor beyond yield is non increasing. The multimaterial integration scheme is based on a simple numerical flux function that keeps the interfaces sharp. Numerical illustrations in one to three space dimensions of high-speed multimaterial impacts in air are presented.

In TC4 an iron sphere is impacting an aluminium plate immersed in air. The computational domain is $[-0.3, 0.7] \times [-0.4, 0.4] \times [-0.4, 0.4]$m. The initial velocity of the projectile is $1000 m.s^{-1}$. The computation is performed on a $500 \times 400 \times 400$ mesh with 216 processors. Homogeneous Neumann conditions are imposed on the left and right borders and cantilever on the others.

The results are given in Fig 17 where we present the Schlieren results on the vertical symmetry plane and the material interfaces. As in the 2D case the projectile perforates the aluminium plate which is strongly stretched. The breaking of the plate at final time is due to the level set function resolution.

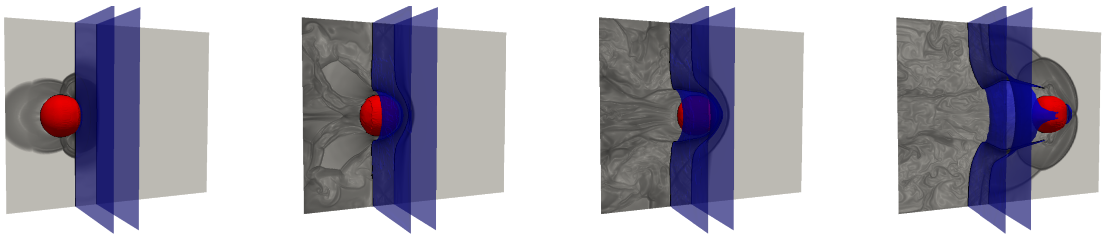


Figure 17. Schlieren representation on the vertical symmetry plane and the material interfaces.

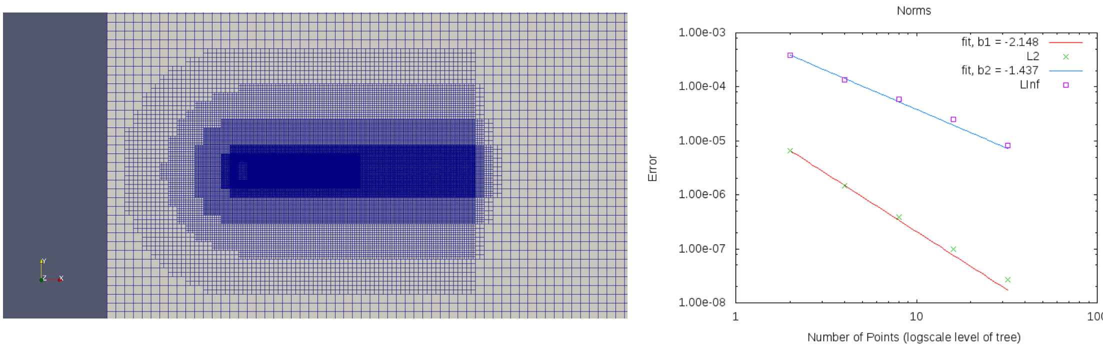
7.7. Hierarchical grids: applications with quadtrees/octrees

A first application with a specific method is the resolution of the incompressible Navier-Stokes equations. A Navier-Stokes solver dealing with quadtrees has been implemented in parallel this year. The overall aim will be to model in 3D the flow over a wind turbine using an Octree grid. On the figure 18 can be seen an example of QuadTree mesh. A Finite Volume Semi-Lagrangian scheme is used.

First, the order of convergence of the Laplacian Solver discretization on QuadTrees has been computed and compared with those obtained with other schemes as explained previously. The method for solving the Laplacian Solver is named Diamond method and consists in using a dual mesh and considering that the Gradients are constants inside. The order of convergence of 2 has been obtained. The order of convergence of the overall Navier-Stokes resolution on QuadTree meshes has been computed and the order of 2 is get as can be seen on figures 18 . For the L_∞ norm, the order of 2 can't be reach caused by the loss of accuracy when a gap in refinement level occurs.

For now the grid is fixed, so the next step will be to refine and coarsen the grid following the position of the obstacle and the "interesting" areas. The work will then go on with the implementation of this Navier-Stokes solver with adaptive QuadTree meshes in 3D.

A second application is phase changing material. We consider problems governed by linear elliptic equations with discontinuity interfaces across the domain. The equation coefficients, the solution and its normal



(a) Example of QuadTree mesh for circular cylinder (b) Norms as a function of number of points on grid

Figure 18.

derivative can undergo a jump across these internal boundaries. We present a compact second-order finite-difference scheme on a tree-based adaptive grid that can be efficiently solved in parallel. The main idea is to optimize the truncation error of the discretization as a function of the local grid configuration.

The variable coefficient heat diffusion problem we consider is modeled by:

$$-\text{div}(\kappa(\overrightarrow{x})\nabla u(\overrightarrow{x})) = g(\overrightarrow{x}), \quad \text{in } D, \tag{2}$$

$$R(\kappa \partial_{\overrightarrow{n}} u(\overrightarrow{x}))_S = [u], \text{ on } \gamma \tag{3}$$

$$[\kappa(\overrightarrow{x})\partial_{\overrightarrow{n}} u(\overrightarrow{x})] = 0, \quad \text{on } \gamma \tag{4}$$

Where $\overrightarrow{x} = (x, y, z)$ are the spatial coordinates and $\kappa(\overrightarrow{x})$ is piecewise continuous on each subdomain but it may be discontinuous across γ (the boundary of the D subdomain that contains the discontinuities through). A cell-centered investigation often leads to a symmetric linear system, since the relation between two neighbors is reflective. Considering the configuration in Fig. 19 it is natural to define the discretization at c_4 in terms of the others.

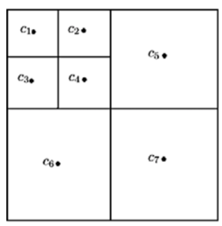


Figure 19. A test configuration centerd in c_4.

Let h be the side length of the cell c_4. To obtain the existence of a linear consistent scheme we must be able to find the coefficients a_i such that:

$$u_{xx} + u_{yy} = a_1u_1 + a_2u_2 + a_3u_3 + a_4u_4 + a_5u_5 + a_6u_6 + a_7u_7 + O(h)$$

A complete Taylor's analysis on all the involved neighbors, applying them relative linear combinations of the expansions, implies that the coefficients a_i must satisfy the following linear system:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -h & 0 & -h & \frac{3h}{2} & -\frac{h}{2} & \frac{3h}{2} \\ 0 & h & h & 0 & \frac{h}{2} & -\frac{3h}{2} & -\frac{3h}{2} \\ 0 & \frac{h^2}{2} & 0 & \frac{h^2}{2} & \frac{9h^2}{8} & \frac{h^2}{8} & \frac{9h^2}{8} \\ 0 & -h^2 & 0 & 0 & \frac{3h^2}{4} & \frac{3h^2}{4} & -\frac{9h^2}{4} \\ 0 & \frac{h^2}{2} & \frac{h^2}{2} & 0 & \frac{h^2}{8} & \frac{9h^2}{8} & \frac{9h^2}{8} \end{pmatrix} \begin{pmatrix} a_4 \\ a_1 \\ a_2 \\ a_3 \\ a_5 \\ a_6 \\ a_7 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

In the example above there are seven concerned points, so, we can determine infinite solutions of the complete system but we search a unique one. Let M be the constraints matrix, $\overrightarrow{a}$ the weights vector, $\overrightarrow{f}$ the right hand side vector for consistency and $F(\overrightarrow{a})$ a weights function. The problem to minimize has the Lagrangian form:

$$\mathcal{L} = F(\overrightarrow{a}) - \overrightarrow{\lambda}(M\overrightarrow{a} - \overrightarrow{f}) \tag{5}$$

We write the minimization problem (5) in matrix form like:

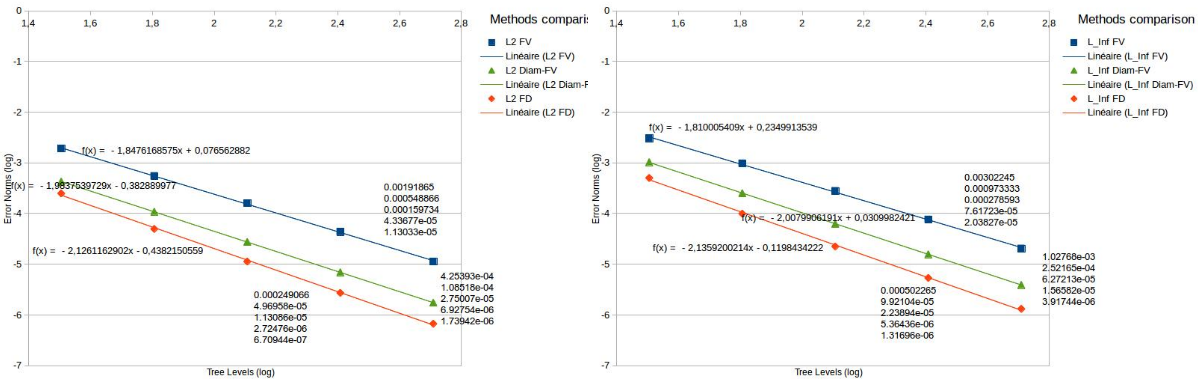
$$Ax = b \Leftrightarrow \begin{cases} \frac{\partial F(\overrightarrow{a})}{\partial \overrightarrow{a}} - M^T\overrightarrow{\lambda} & = 0 \\ M\overrightarrow{a} & = \overrightarrow{f} \end{cases}$$

This choice allows us to implement a scheme always consistent case by case.

Following a consistence proof several tests have been produced to strenghten our method like penalization and different kinds of model until a modeling of the problem (7.7) step by step. We built a new cell centered finite difference method able to:

- be consistent and locally convergent to second order on balanced grids;
- simplify and promote an AMR approach along discontinuity;
- solve the coupled problems (2)-(3) and (2)-(4);
- a first consistent result on the complete model (2)-(3)-(4).

The finite different method presented here has been compared with two other methods finite volume scheme (Fig. 20). The first one has been implemented by Marco Cisternino and the diamonds one by Claire Taymans (see previous sections). All the three methods stick on the same grid and they use PABLO's data structure with its parallel balance.



(a) L_2 norm comparison (b) L_∞ norm comparison

Figure 20. Comparison between several numerical approaches.

MEPHYSTO Project-Team

7. New Results

7.1. Macroscopic behaviors of large interacting particle systems

7.1.1. Stochastic acceleration and approach to equilibrium

S. De Bièvre, Carlos Mejia-Monasterio (Madrid) and Paul E. Parris (Missouri) [57] studied thermal equilibration in a two-component Lorentz gas, in which the obstacles are modeled by rotating disks. They show that a mechanism of dynamical friction leads to a fluctuation-dissipation relation that is responsible for driving the system to equilibrium.

Stephan De Bièvre, Jeremy Faupin (Metz) and Schuble (Metz) [59] studied a related model quantum mechanically. Here a quantum particle moves through a field of quantized bose fields, modeling membranes that exchange energy and momentum with the particle. They establish a number of spectral properties of this model, that will be essential to study the time-asymptotic behavior of the system.

S. De Bièvre and collaborators analyse in [20] a multi-particle, kinetic version of a Hamiltonian model describing the interaction of a gas of particles with a vibrating medium. They prove existence results for weak solutions, and identify an asymptotic regime where the model, quite surprisingly, approaches the attractive Vlasov—Poisson system.

7.1.2. Towards the weak KPZ universality conjecture

One may start by considering the microscopic system in equilibrium (its measure is parametrized by the thermodynamical quantities under investigation). By removing the mean to the empirical measure and by scaling it properly, one would like to show that the random process, obtained by this rescaling, converges, as the size of the system is taken to infinity, to another random process which is a solution of some generalized stochastic PDE. Thanks to the remarkable recent result of M. Jara and P. Gonçalves [66], one has now all in hands to establish the latter result for a particular stochastic PDE known as the stochastic Burgers equation, and its companion, the Kardar-Parisi-Zhang (KPZ) equation. Indeed, in the latter paper, the authors introduce a new tool, called the second order Boltzmann-Gibbs principle, which permits to replace certain additive functionals of the dynamics by similar functionals given in terms of the density of the particles.

In [28], M. Simon in collaboration with T. Franco and P. Gonçalves, investigate the case of a microscopic dynamics with local defects, which is much harder. More precisely, the microscopic particle system is locally perturbed, and depending on the type of perturbation, the macroscopic laws can hold different boundary conditions. Since the ideas of [66] do not apply to the model considered there, they propose a new way to estimate the error in the replacement performed in the Boltzmann-Gibbs principle.

In the same spirit, M. Simon in collaboration with O. Blondel and P. Gonçalves investigate in [7] the class of kinetically constrained lattice gases that have been introduced and intensively studied in the literature in the past few years. In these models, particles are subject to restrictive constraints that make both approaches of [66] and [28] not work, so that new mathematical tools are needed. The main technical difficulty is that their model exhibits configurations that do not evolve under the dynamics and are locally non-ergodic. Their proof does not impose any knowledge on the spectral gap for the microscopic models. Instead, it relies on the fact that, under the equilibrium measure, the probability to find a blocked configuration in a finite box is exponentially small in the size of the box.

With these two recent results, M. Simon and coauthors contribute towards the *weak KPZ universality conjecture*, which states that a large class of one-dimensional weakly asymmetric conservative systems should converge to the KPZ equation.

7.1.3. Diffusion and fractional diffusion of energy

The rigorous derivation of the heat equation from deterministic systems of Newtonian particles is one of the most fundamental questions in mathematical physics. The main issue is that the existence of conservation laws and the high number of degrees of freedom impose very poor ergodic properties to the associated dynamical systems. A possible way out of this lack of ergodicity is to introduce stochastic models, in such a way that in one hand ergodicity issues are solved by the stochastic dynamics and in the other hand the qualitative behaviour of the system is not modified by the randomness. In these models, one starts with a chain of oscillators with a Hamiltonian dynamics, and one adds a stochastic component in such a way that the fundamental conservation laws (energy, momentum and *stretch* in this case) are maintained, and the corresponding Gibbs measures become ergodic.

It was already proved in [51] that these stochastic chains model correctly the behaviour of the conductivity. In particular, it is prove that Fourier law holds in dimension $d \geq 3$ if energy and momentum are conserved, and in any dimension if only energy is conserved. Once the conductivity has been successfully understood, one investigates the existence of the *hydrodynamic limit*, which fully describes the macroscopic evolution of the *empirical profiles* associated to the conserved quantity. In [41], M. Simon in collaboration with T. Komorowski and S. Olla consider the unpinned harmonic chain where the velocities of particles can randomly change sign. The only conserved quantities of the dynamics are the energy and the elongation. Using a diffusive space-time scaling, the profile of elongation evolves independently of the energy and follows a linear diffusive equation. The energy profile evolves following a non-linear diffusive equation involving the elongation. The presence of non-linearity makes the macroscopic limit non-trivial, and its mathematical proof requires very sophisticated arguments.

In [52] and [69] it has been previously shown that in the case of one-dimensional harmonic oscillators with noise that preserves the momentum, the scaling limit of the energy fluctuations is ruled by the *fractional* heat equation

$$\partial_t u = -(-\Delta)^{3/4} u.$$

This equation does not only predict the superdiffusivity of energy in momentum-conserving models, but it also predicts the speed at which it diverges. This result opens a way to a myriad of open problems. The main goal is to observe anomalous fractional superdiffusion type limit in the context of low dimensional asymmetric systems with several conserved quantities. In two recent papers by M. Simon in collaboration with C. Bernardin, P. Gonçalves, M. Jara, M. Sasada [53] & [32], they confirmed rigorously recent Spohn's predictions on the Lévy form of the energy fluctuations for a harmonic chain perturbed by an energy-volume conservative noise. In [32] they also showed the existence of a crossover between a normal diffusion regime and a fractional superdiffusion regime by tuning a parameter of a supplementary stochastic noise conserving the energy but not the volume.

7.2. Qualitative results in homogenization

7.2.1. Isotropy and loss of ellipticity in periodic homogenization

Since the seminal contribution of Geymonat, Müller, and Triantafyllidis, it is known that strong ellipticity is not necessarily conserved by homogenization in linear elasticity. This phenomenon is typically related to microscopic buckling of the composite material. In [24] G. Francfort and A. Gloria study the interplay between isotropy and strong ellipticity in the framework of periodic homogenization in linear elasticity. Mixtures of two isotropic phases may indeed lead to loss of strong ellipticity when arranged in a laminate manner. They show that if a matrix/inclusion type mixture of isotropic phases produces macroscopic isotropy, then strong ellipticity cannot be lost.

7.2.2. From polymer physics to nonlinear elasticity

OIn [23], M. Duerinckx and A. Gloria succeeded in relaxing one of the two unphysical assumptions made in [1] on the growth of the energy of polymer chains. In particular, [23] deals with the case when the energy of the polymer chain is allowed to blow up at finite deformation.

7.2.3. The Clausius-Mossotti formula

In the mid-nineteenth century, Clausis, Mossotti and Maxwell essentially gave a first order Taylor expansion for (what is now understood as) the homogenized coefficients associated with a constant background medium perturbed by diluted spherical inclusions. Such an approach was recently used and extended by the team MATHERIALS to reduce the variance in numerical approximations of the homogenized coefficients, cf. [46], [45], [72]. In [22], M. Duerinckx and A. Gloria gave the first rigorous proof of the Clausius-Mossotti formula and provided the theoretical background to analyze the methods introduced in [72].

7.3. Quantitative results in stochastic homogenization

7.3.1. Quantitative results for almost periodic coefficients

In [6], S. Armstrong, A. Gloria and T. Kuusi (Aalto University) obtained the first improvement over the thirty year-old result by Kozlov [70] on almost periodic homogenization. In particular they introduced a class of almost periodic coefficients which are not quasi-periodic (and thus strictly contains the Kozlov class) and for which almost periodic correctors exist. Their approach combines the regularity theory developed by S. Armstrong and C. Smart in [49] and adapted to the almost periodic setting by S. Armstrong and Z. Shen [48], a new quantification of almost-periodicity, and a sensitivity calculus in the spirit of [3].

7.3.2. Optimal stochastic integrability in stochastic homogenization

In [40] A. Gloria and F. Otto consider uniformly elliptic coefficient fields that are randomly distributed according to a stationary ensemble of a finite range of dependence. They show that the gradient and flux $(\nabla\phi, a(\nabla\phi + e))$ of the corrector ϕ, when spatially averaged over a scale $R \gg 1$ decay like the CLT scaling $R^{-d/2}$. They establish this optimal rate on the level of *sub-Gaussian* bounds in terms of the stochastic integrability, and also establish a suboptimal rate on the level of optimal Gaussian bounds in terms of the stochastic integrability. The proof unravels and exploits the self-averaging property of the associated semi-group, which provides a natural and convenient disintegration of scales, and culminates in a propagator estimate with strong stochastic integrability. As an application, they characterize the fluctuations of the homogenization commutator, and prove sharp bounds on the spatial growth of the corrector, a quantitative two-scale expansion, and several other estimates of interest in homogenization.

7.3.3. A theory of fluctuations in stochastic homogenization

In [39], M. Duerinckx, A. Gloria, and F. Otto establish a path-wise theory of fluctuations in stochastic homogenization of linear elliptic equations in divergence form. More precisely they consider the model problem of a discrete equation with independent and identically distributed conductances (as considered in [27]). They identify a single quantity, which they call the homogenization commutator, that drives the fluctuations in stochastic homogenization in the following sense. On the one hand, this tensor-valued stationary random field satisfies a functional central limit theorem, and (when suitably rescaled) converges to a Gaussian white noise. On the other hand, the fluctuations of the gradient of the corrector, the fluctuations of the flux of the corrector, and the fluctuations of any solution of the PDE with random coefficients and localized right-hand side are characterized at leading order by the fluctuations of this homogenization commutator in a path-wise sense. As a consequence, when properly rescaled, the solution satisfies a functional central limit theorem, the gradient of the corrector converges to the Helmholtz projection of a Gaussian white noise, and the flux of the corrector converges to the Leray projection of the same white noise. Compared to previous contributions, our approach, based on the homogenization commutator, unravels the complete structure of fluctuations. It holds in any dimension $d \geq 2$, yields the first path-wise results, quantifies the limit theorems in Wasserstein distance, and only relies on arguments that extend to the continuum setting and to the case of systems.

7.4. Numerical methods for evolution equations

In [36] G. Dujardin analyzes an exponential integrator applied to the nonlinear Schrödinger equation with white noise dispersion. This models appears in optic fibers. Together with his co-author, he proves that this explicit scheme applied to the sctochastic PDE is of mean-square order 1. He uses it to illustrate a conjecture on the well-posedness of the equation in some regimes of the nonlinearity. Comparisons with several other schemes of the litterature are proposed. A last, another new (implicit) exponential integrators is proposed, which preserves the L^2-norm of the solution and is compared with the explicit one introduced beforehand.

7.5. Schrödinger equations

7.5.1. Nonlinear optical fibers

S. Rota Nodari, G. Dujardin, S. De Bièvre and collaborators continued their previous work on periodically modulated optical fibers with the experimental physicists of PhLAM [19]. They show that the nonlinear stage of modulational instability induced by parametric driving in the *defocusing* nonlinear Schrödinger equation can be accurately described by combining mode truncation and averaging methods, valid in the strong driving regime. The resulting integrable oscillator reveals a complex hidden heteroclinic structure of the instability. A remarkable consequence, validated by the numerical integration of the original model, is the existence of breather solutions separating different Fermi-Pasta-Ulam recurrent regimes.

In [42] S. de Bièvre and G. Dujardin analyze the formation of the Kuznetsov-Ma soliton of the 1D Schrödinger equation in the presence of periodic modulation satisfying an integrability condition. They show that this particular soliton has several compression points, the number, position and shape of which are controlled by the amplitude and the frequency of the modulation. They analyze the interplay between the frenquency of the soliton and the frequency of the modulation. Moreover, they show that one can suppress any component of the output spectrum of the soliton by a suitable choice of the amplitude and frequency of the modulation.

These works are part of the activities developped in the LabEx CEMPI.

7.5.2. Nonlinear Schrödinger equations

In [54], D. Bonheure, J.-B. Casteras and R. Nascimento obtained new results on the existence and qualitative properties of waveguides for a mixed-diffusion NLS. In particular, they proved the first existence results for waveguides with fixed mass and provided several qualitative descriptions of these.

S. De Bièvre and S. Rota Nodari continued their work on orbital stability of relative equilibria of Hamiltonian dynamical systems on Banach spaces, with a second paper [37], dealing with the situation where multi-dimensional invariance groups are present in the systems considered. They present a generalization of the Vakhitov-Kolokolov slope condition to this higher dimensional setting, and show how it allows to prove the local coercivity of the Lyapunov function, which in turn implies orbital stability. The method is applied to study the orbital stability of the plane waves of a system of two coupled nonlinear Schrödinger equations. They provide a comparison of their approach to the classical one by Grillakis-Shatah-Strauss.

7.6. Miscellaneous results

In [21] Mitia Duerinckx establishes the global well-posedness of a family of equations, which are obtained in certain regimes — in a joint work in preparation with Sylvia Serfaty — as the mean-field evolution of the supercurrent density in a (2D section of a) type-II superconductor with pinning and with imposed electric current. General vortex-sheet initial data are also considered, and the uniqueness and regularity properties of the solution are investigated.

In [33], [8], [11], [12], D. Bonheure, J.-B. Casteras and collaborators made bifurcation analysis and constructed multi-layer solutions of the Lin-Ni-Takagi and Keller-Segel equations, which come from the Keller-Segel system of chemotaxis in specific cases. A remarkable feature of the results is that the layers do not accumulate to the boundary of the domain but satisfy an optimal partition problem contrary to the previous type of solutions constructed for these models.

In [16], [17], [35], J.-B. Casteras and collaborators study different problems related to the existence of constant mean curvature hypersurfaces with prescribed asymptotic boundary on Cartan-Hadamard manifold. In particular, they obtained the first existence results for minimal graphs with prescribed asymptotic Dirichlet data under a pointwise pinching condition for sectionals curvatures.

S. De Bièvre and co-workers present in [67] a general approach to calculating the entanglement of formation for superpositions of two-mode coherent states, placed equidistantly on a circle in phase space. In the particular case of rotationally-invariant circular states the value of their entanglement is shown to be given by analytical expressions. They analyse the dependence of the entanglement on the radius of the circle and number of components in the superposition.

A. Benoit continues his analysis of hyperbolic equations in corner spaces. He addresses in [30] the rigorous construction of geometric optics expansions for weakly well-posed hyperbolic corner problems. He studies in [31] the semi-group stability for finite difference discretizations of hyperbolic systems of equations in corner domains, extending previous results of Coulombel & Gloria and Coulombel in the case of the halfspace.

MOKAPLAN Project-Team

7. New Results

7.1. Inverse problems with sparsity prior

G. Peyré, V. Duval, Q. Denoyelle,C. Poon

In [12], we have studied the stability of a classical image processing method, the Total Variation (TV) Denoising model introduced by Rudin, Osher and Fatemi [171]. While TV denoising is a well studied problem, our contribution is one of the first to address the impact of noise on the solutions. We have shown that the level lines of the denoised image (hence the edges and the gradient of shades) are located near an area called “extended support” which depends on the curvature of the image to recover. This yields a precise description of the so-called “staircasing” effect which is characteristic of the method, as well as the support stability of the method (see Figure 12). In particular, we have proved that indicator functions of calibrable sets are stable to noise, in the sense that the level lines of the denoised image will be close to the boundary of the original set.

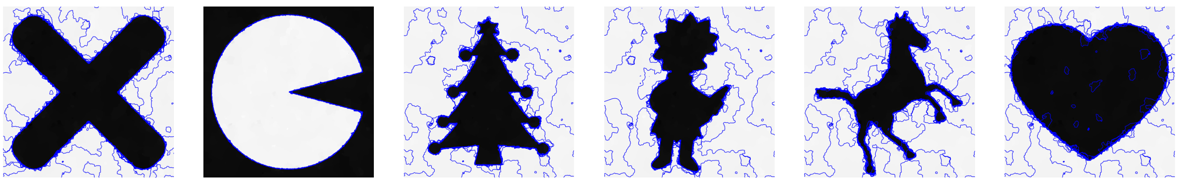


Figure 12. Level lines of denoised images with low regularization (TV denoising)

In [38], we have studied the problem of recovering a sparse signal (say, a sum of Dirac masses), from its blurred, partial, Radon transform, or equivalently by sampling the low frequency coefficients of its Fourier transform along a few radial lines. We have proved that, using a total variation (of measures) regularization approach in the spirit of [96], one may reconstruct exactly the signal under some geometric condition, or, in a compressed sensing approach, with high probability if one subsamples the coefficients. We propose a numerical algorithm to exactly solve this problem, by a converting it to a few low-dimensional Semi-Definite Programs.

7.2. Mean Field Games and augmented lagrangian methods for optimal transport

Roman Andreev

We apply the augmented Lagrangian method to the convex optimization problem of the instationary variational mean field games with diffusion. The system is first discretized with space-time tensor product piecewise polynomial bases. This leads to a sequence of linear problems posed on the space-time cylinder that are second order in the temporal variable and fourth order in the spatial variable. To solve these large linear problems with the preconditioned conjugate gradients method we propose a parameter-robust preconditioner that is based on a temporal transformation coupled with a spatial multigrid. Numerical examples illustrate the method. [27].

G. Carlier J-D. Benamou have written in collaboration with F. Santambrogio a review paper on variational MFG [31] both on theoretical and numerical aspects, the latter being addressed by augmented Lagrangian techniques developed by our team also in the context of optimal transport for an arbitrary Finsler metric cost [30] (the main advantage of our method being that we never have to evaluate the cost).

7.3. Gromov-Wasserstein methods in graphics and machine learning

G. Peyré, J. Solomon, M. Cuturi

A bottleneck of optimal transport (OT) methods for some applications in graphics and machine learning is that it requires the knowledge of an a priori fixed ground cost. This cost is often chosen as some power of a distance, which in turn requires that the data to compare or modify are pre-registered in a common embedding metric space (e.g. the 3-D or 2-D Euclidean space for shapes matching). For many applications (such a shape matching in vision or molecule comparison in quantum chemistry), this is simply not the case. We thus propose in [18], [21] to extend the computational machinery of OT to cope with an unknown cost by using the so-called Gromov-Wasserstein distance. This distance allows to compare probability distributions living in *different* and un-registered metric spaces, by coupling together pairs of points instead of single points. This allows to formulate a non-convex energy minimization, which is similar to the graph matching problem. We propose to use the entropic regularization scheme to solve it numerically, and we showed that it leads to a very effective Sinkhorn-like algorithm. In [18] (published in SIGGRAPH, the best computer graphics conference) we explore various application in computer graphics (such as shape matching or organization of collections of surfaces and images), while [21] (published in ICML, one of the two best machine learning conference) we extend this machinery to compute interpolation and barycenter of several metric space, with application to shape interpolation and supervised learning for quantum chemistry.

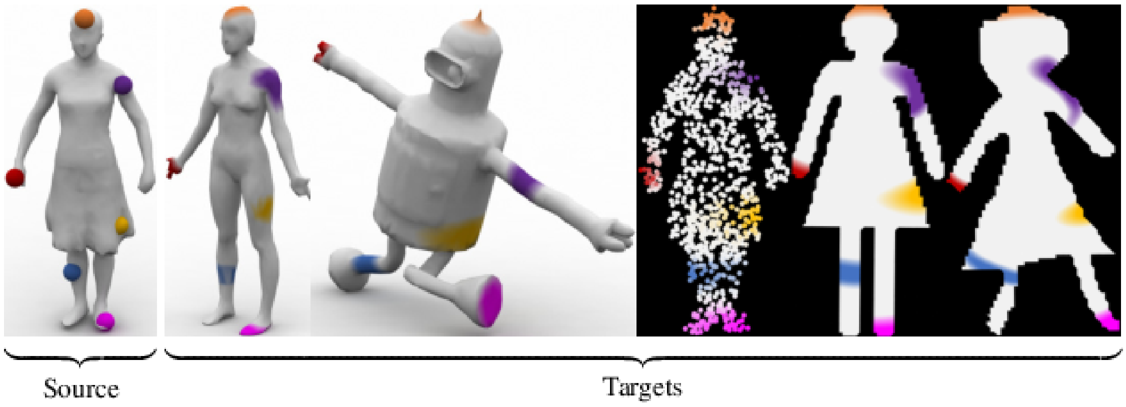


Figure 13. Example of matching induced between an input 3-D shape (on the left) and 3-D or 2-D shapes using the transport coupling computed using our entropy-regularized Gromov-Wasserstein problem. From [18].

7.4. Optimal transport meets machine learning

A. Genevay, G. Peyré, M. Cuturi, F. Bach

Optimal transport has recently proved (in particular through the works of our team) to be very successful to solve various low dimensional problems, mostly in 2-D and 3-D. These successes are mainly due to the specicfic structure of these problems (the connections with PDE's and the use of entropic regularization), but these approaches do not scale to high dimensional and large scale problems that one encounters in machine learning. In these problems, it is not possible to discretize the space, and one does not have a direct access to the density to compare. One can rather only *sample* from these distributions. To address these difficulties, we propose in [20] (published in NIPS, one of the best two machine learning conferences), the first provably convergent algorithm that can cope with high dimensional OT problems, with both discrete and continuous input measures. This approach leverage both the structure of the dual problem, and the smoothness induced by an entropic regularization. We show application of this method for classification of high dimensional bag of features histograms.

7.5. Optimal Transportation numerical methods for Fluid models

F-X. Vialard Q. Mérigot L. Nenna G. Carlier J-D. Benamou

Several new algorithms based on Optimal Transport have applied to Generalized Euler Geodesics and the Cauchy problem for the Euler equation. The methods rely on the generalized polar decomposition of Brenier, numerically implemented whether through semi-discrete optimal transport or through entropic regularization. It is robust enough to extract non-classical, multi-valued solutions of Euler's equations predicted by Brenier and Schnirelman. The semi-discrete approach also leads to a numerical scheme able to approximate regular solutions to the Cauchy problem for Euler equations. See Luca Nenna Thesis and [15].
A new link between optimal transport and fluid dynamic was discovered in [42]. Since the work of Brenier, optimal transport is tightly linked with the incompressible Euler equation and can be seen as a nonlinear extension of the pressure. Recently, a new optimal transport model between unbalanced measures has been proposed by some of the members of Mokaplan. In [41], it is shown that the corresponding fluid dynamic equation is the Camassa-Holm equation, well known to model waves in shallow water and wave breaking. On the theoretical side, we prove that the solutions to the Camassa-Holm equation can be seen as particular solutions of the incompressible Euler equation. This work paves the way for the study of the generalized Camassa-Holm geodesics and numerical methods based on unbalanced optimal transport scaling algorithms to solve it.

7.6. Scaling Algorithms and OT

G. Peyré F-X. Vialard L. Chizat B. Schmitzer S. Di Marino

B. Schmitzer has developed a sparse solver based on entropic regularization and numerical methods to solve unbalanced optimal transport (developed by our team in 2015) have been proposed in [37]. The core of the method consists in using the entropy functional as a reguflarizer and a barrier method. This is a generalization of the Sinkhorn method that has been introduced recently by M. Cuturi in numerical optimal transport. One important contribution of this work is to give a unified formulation of unbalanced optimal transport that can address a whole range of possible metrics and encompasses different applications such as Karcher-Fréchet averages, gradient flows, multimarginal unbalanced optimal transport. These two works are essentially based on a log-domain stabilized formulation, an adaptive truncation of the kernel and a coarse-to-fine scheme. This allows to solve large problems where the regularization is almost negligible.
In particular, this scaling algorithm is applied in its gradient flow formulation in the unbalanced case to obtain accurate simulations of the Hele-Shaw model, which models the cancer tumor growth.

7.7. Optimal transport meets economics

G. Carlier J-D. Benamou L. Nenna, G. De Bie

G. Carlier and L. Nenna in collaboration with Adrien Blanchet [32] developed an entropic-regularization scheme to compute Cournot Nash equilibria (i.e. equilibria in games with a continuum of players) for generic costs. With Lina Mallozzi, G. Carlier [36] introduced a partial optimal mass transport approach for spatial monopoly pricing both in the deterministic and stochastic cases. G. Carlier, J-D. Benamou and X. Dupuis developed various numerical strategies for solving the principal-agent problem in the framework of optimal pricing. Carlier, Chernozhukov and Galichon [34] studied multivariate quantile regression by optimal transport and duality techniques beyond the specified case, Gwendoline de Bie implemented these ideas by entropic regularization.

NACHOS Project-Team

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. Numerical study of the non-linear Maxwell equations for Kerr media

Participants: Loula Fezoui, Stéphane Lanteri.

The system of Maxwell equations describes the evolution of the interaction of an electromagnetic field with a propagation medium. The different properties of the medium, such as isotropy, homogeneity, linearity, among others, are introduced through *constitutive laws* linking fields and inductions. In the present study, we focus on non-linear effects and address non-linear Kerr materials specifically. In this model, any dielectric may become non-linear provided the electric field in the material is strong enough. As a first setp, we considered the one-dimensional case and study the numerical solution of the non-linear Maxwell equations thanks to DG methods. In particular, we make use of an upwind scheme and limitation techniques because they have a proven ability to capture shocks and other kinds of singularities in the fluid dynamics framework. The numerical results obtained in this preliminary study gave us confidence towards extending them to higher spatial dimensions. This year, we have completed the development of a first version a parallel DGTD solver for the three-dimensional based on our past contributions on DGTD methods for the case of linear propagation media.

6.1.2. Numerical treatment of non-local dispersion for nanoplasmonics

Participants: Stéphane Lanteri, Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.

When metallic nanostructures have sub-wavelength sizes and the illuminating frequencies are in the regime of metal's plasma frequency, electron interaction with the exciting fields have to be taken into account. Due to these interactions, plasmonic surface waves can be excited and cause extreme local field enhancements (surface plasmon polariton electromagnetic waves). Exploiting such field enhancements in applications of interest requires a detailed knowledge about the occurring fields which can generally not be obtained analytically. For the numerical modeling of light/matter interaction on the nanoscale, the choice of an appropriate model is a crucial point. Approaches that are adopted in a first instance are based on local (no interaction between electrons) dispersion models e.g. Drude or Drude-Lorentz. From the mathematical point of view, these models lead to an additional ordinary differential equation in time that is coupled to Maxwell's equations. When it comes to very small structures in a regime of 2 nm to 25 nm, non-local effects due to electron collisions have to be taken into account. Non-locality leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. In this work, we study a DGTD method able to solve the system of Maxwell equations coupled to a linearized non-local dispersion model relevant to nanoplasmonics. This year, we have developed a parallel DGTD solver for the three-dimentional Maxwell equations coupeld to a non-local Drude model. Both centered flux-based and upwind flux-based DG schemes have been considered, in combination with with leap-frog and Runge-Kutta time stepping respectively.

6.1.3. Corner effects in nanoplasmonics

Participants: Camille Carvalho [ENSTA, POEMS project-team], Patrick Ciarlet [ENSTA, POEMS project-team], Claire Scheid.

In this work, we study nanoplasmonic structures with corners (typically a diedral/truangular structure). This is the central subject considered in the PhD thesis of Camille Carvalho. In the latter, the focus is made on a lossles Drude dispersion model with a frequency-domain approach. Several well posedness problems arise due to the presence of corners and are addressed in the PhD thesis. A time-domain approach in this context is also relevant and we propose to use the techniques developed in the team in this prospect. Even if both approaches (time-domain and frequency-domain) represent similar physical phenomena, problems that arise are different. These two approaches appear as complementary; it is thus worth bridging the gap between the two frameworks. We are currently performing a thorough comparison in the case of theses 2D structures with corners and we especially focus on the amplitude principle limit that raises a lot of questions.

6.1.4. Travelling waves for the non-linear Schrödinger equation in 2D

Participants: David Chiron [J.A. Dieudonné Laboratory, Université Nice Sophia Antipolis], Claire Scheid, Serge Nicaise [Université de Valenciennes et du Hainaut-Cambrésis], Claire Scheid.

We are interested in the numerical study of the two-dimensional travelling waves of the non-linear Schrödinger equation for a general non-linearity and with nonzero condition at infinity. This equation is appearing in models of nonlinear optics. It has a variational structure that we propose to exploit to design a numerical method. We continue the sudy initiated in [1] and investigate excited states of the Kadomtsev-Petviashvili-I (KP-I) and Gross-Pitaevskii (GP) equations in dimension 2. We address numerically the question of the Morse index of some explicit solutions of KP-I. The results confirm that the lump solitary wave has Morse index one and that the other explicit solutions correspond to excited states. We then turn to the 2D GP equation which in some long wave regime converges to the KP-I equation. We finally perform numerical simulations showing that the other explicit solitary waves solutions to the KP-I equation give rise to new branches of travelling waves of GP corresponding to excited states.

In this ongoing work, we are interested in fundamental properties of the non local linearized hydrodynamic Drude model introduced in the context of nanoplasmonics. We propose an existence and detailed (polynomial/exponential) stability study for these models. We also investigate the discrete stability results. We propose to study the impact of the DG schemes developped in the team on these properties. This study complements the numerical approach that we already propose in the context of the PhD of Nikolai Schmitt for this model, towards a thorough understanding of its fundamentals properties.

6.1.5. A structure preserving numerical discretization framework for the Maxwell Klein Gordon equation in 2D.

Participants: Snorre Christiansen [Department of Mathematics, University of Oslo, Norway], Claire Scheid.

Toward a better understanding of non-linear optical phenomena, we focus on the case of the Maxwell Klein Gordon (MKG) equation in dimension 2. This equation appears in the context of quantum electrodynamics but also in relativity. We propose to develop a numerical discretization framework that takes advantage of the Hamiltonian structure of the equation. The gauge invariance is recovered at the discrete level with the help of the Lattice Gauge theory. We then propose a fully discrete scheme and prove its convergence. The strategy of proof, based on discrete energy principle, is developed in a more general context and next applied in the particular case of MKG equation. This work has been conducted and finalized during a of five month's stay of C. Scheid at the University of Oslo through an invitation in the contexty of the ERC Starting Grant project STUCCOFIELD of S. Christiansen.

6.1.6. Multiscale DG methods for the time-domain Maxwell equations

Participants: Stéphane Lanteri, Raphaël Léger, Diego Paredes Concha [Instituto de Matemáticas, Universidad Católica de Valparaiso, Chile], Claire Scheid, Frédéric Valentin [LNCC, Petropolis, Brazil].

Although the DGTD method has already been successfully applied to complex electromagnetic wave propagation problems, its accuracy may seriously deteriorate on coarse meshes when the solution presents multiscale or high contrast features. In other physical contexts, such an issue has led to the concept of multiscale basis functions as a way to overcome such a drawback and allow numerical methods to be accurate on coarse meshes. The present work, which is conducted in the context of the HOMAR Associate Team, is concerned with the study of a particular family of multiscale methods, named Multiscale Hybrid-Mixed (MHM) methods. Initially proposed for fluid flow problems, MHM methods are a consequence of a hybridization procedure which caracterize the unknowns as a direct sum of a coarse (global) solution and the solutions to (local) problems with Neumann boundary conditions driven by the purposely introduced hybrid (dual) variable. As a result, the MHM method becomes a strategy that naturally incorporates multiple scales while providing solutions with high order accuracy for the primal and dual variables. The completely independent local problems are embedded in the upscaling procedure, and computational approximations may be naturally obtained in a parallel computing environment. In this study, a family of MHM methods is proposed for the solution of the time-domain Maxwell equations where the local problems are discretized either with a continuous FE method or a DG method (that can be viewed as a multiscale DGTD method). Preliminary results have been obtained in the two-dimensional case.

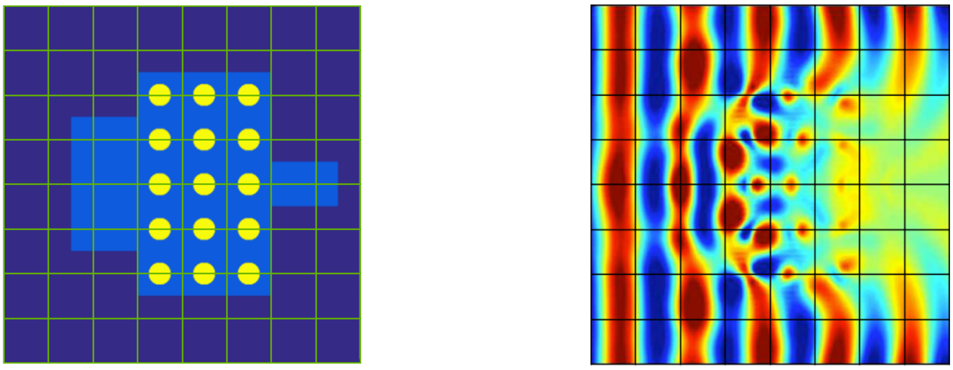


Figure 4. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

6.1.7. HDG methods for the time-domain Maxwell equations

Participants: Alexandra Christophe-Argenvillier, Stéphane Descombes, Stéphane Lanteri.

This study is concerned with the development of accurate and efficient solution strategies for the system of 3D time-domain Maxwell equations coupled to local dispersion models (e.g. Debye, Drude or Drude-Lorentz models) in the presence of locally refined meshes. Such meshes impose a constraint on the allowable time step for explicit time integration schemes that can be very restrictive for the simulation of 3D problems. We consider here the possibility of using an unconditionally stable implicit time or a locally implicit time integration scheme combined to a HDG discretization method.

6.1.8. HDG methods for the frequency-domain Maxwell equations

Participants: Alexis Gobé, Stéphane Lanteri, Ludovic Moya.

In the context of the ANR TECSER project, we continue our efforts towards the development of scalable high order HDG methods for the solution of the system of 3D frequency-domain Maxwell equations. We aim at fully exploiting the flexibiity of the HDG discretization framework with regards to the adaptation of the interpolation order (p-adaptivity) and the mesh (h-adaptivity). In particular, we study the formulation of HDG methods on a locally refined non-conforming tetrahedral mesh and on a non-confoming hybrid cubic/tetrahedral mesh. We also investigate the coupling between the HDG formulation and a BEM (Boundary Element Method) discretization of an integral representation of the electromagnetic field in the case of propagation problems theoretically defined in unbounded domains. The associated methodological contributions are implemented in the HORSE simulation software.

6.1.9. HDG methods for the frequency-domain plasmonics

Participants: Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Asger Mortensen [DTU Fotonik, Technical University of Denmark], Martijn Wubs [DTU Fotonik, Technical University of Denmark].

In this colleaboration with physicists at DTU Fotonik, we study HDG methods for solving the frequency-domain Maxwell's equations coupled to the Nonlocal Hydrodynamic Drude (NHD) and Generalized Nonlocal Optical Response (GNOR) models, which are employed to describe the optical properties of nanoplasmonic scatterers and waveguides. The formulations of the HDG method for these two models are exetnsion of our previous works for classical microwave applications. In teh present case, two conservativity conditions are globally enforced to make the problem solvable and to guarantee the continuity of the tangential component of the electric field and the normal component of the current density. Numerical results show that the proposed HDG methods converge at optimal rate. These new HDG formulations hace been implemented and numerically assessed for two-dimensional problems.

6.1.10. Exponential time integrators for a DGTD method

Participants: Stéphane Descombes, Stéphane Lanteri, Bin Li [UESTC, Chengdu, China], Hao Wang [UESTC, Chengdu, China], Li Xu [UESTC, Chengdu, China].

The objective of this study is to design efficient and (high order) accurate time integration strategies for the system of time-domain Maxwell equations discretized in space by a high order discontinuous Galerkin scheme formulated on locally refined unstructured meshes. A new family of implicit-explicit (IMEX) schemes using exponential time integration is developed. The Lawson procedure is applied based on a partitioning of the underlying tetrahedral mesh in coarse and fine parts, allowing the contruction of a time advancing strategy that combines an exact integration of the semi-discrete system for the problem unknowns associated to the elements of the fine part, with an arbitrary high order explicit time integration scheme for the Lawson-transformed system.

6.2. Elastodynamic wave propagation

6.2.1. HDG method for the frequency-domain elastodynamic equations

Participants: Hélène Barucq [MAGIQUE-3D project-team, Inria Bordeaux - Sud-Ouest], Marie Bonnasse, Julien Diaz [MAGIQUE-3D project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

One of the most used seismic imaging methods is the full waveform inversion (FWI) method which is an iterative procedure whose algorithm is the following. Starting from an initial velocity model, (1) compute the solution of the wave equation for the N sources of the seismic acquisition campaign, (2) evaluate, for each source, a residual defined as the difference between the wavefields recorded at receivers on the top of the subsurface during the acquisition campaign and the numerical wavefields, (3) compute the solution of the wave equation using the residuals as sources, and (4) update the velocity model by cross correlation of images produced at steps (1) and (3). Steps (1)-(4) are repeated until convergence of the velocity model is achieved. We then have to solve $2N$ wave equations at each iteration. The number of sources, N, is usually large (about 1000) and the efficiency of the inverse solver is thus directly related to the efficiency of the numerical method used to solve the wave equation. Seismic imaging can be performed in the time-domain or in the frequency-domain regime. In this work which is conducted in the framework of the Depth Imaging Partnership (DIP) between Inria and TOTAL, we adopt the second setting. The main difficulty with frequency-domain inversion lies in the solution of large sparse linear systems which is a challenging task for realistic 3D elastic media, even with the progress of high performance computing. In this context, we study novel high order HDG methods formulated on unstructured meshes for the solution of the frency-domain elastodynamic equations. Instead of solving a linear system involving the degrees of freedom of all volumic cells of the mesh, the principle of a HDG formulation is to introduce a new unknown in the form of Lagrange multiplier representing the trace of the numerical solution on each face of the mesh. As a result, a HDG formulation yields a global linear system in terms of the new (surfacic) unknown while the volumic solution is recovered thanks to a local computation on each element.

6.2.2. Multiscale DG methods for the time-domain elastodynamic equations

Participants: Marie-Hélène Lallemand, Raphaël Léger, Frédéric Valentin [LNCC, Petropolis, Brazil].

In the context of the visit of Frédéric Valentin in the team, we have initiated a study aiming at the design of novel multiscale methods for the solution of the time-domain elastodynamic equations, in the spirit of MHM (Multiscale Hybrid-Mixed) methods previously proposed for fluid flow problems. Motivation in that direction naturally came when dealing with non homogeneous anisotropic elastic media as those encountered in geodynamics related applications, since multiple scales are naturally present when high contrast elasticity parameters define the propagation medium. Instead of solving the usual system expressed in terms of displacement or displacement velocity, and stress tensor variables, a hybrid mixed-form is derived in which an additional variable, the Lagrange multiplier, is sought as representing the (opposite) of the surface tension defined at each face of the elements of a given discretization mesh. We consider the velocity/stress formulation of the elastodynamic equations, and study a MHM method defined for a heterogeneous medium where each elastic material is considered as isotropic to begin with. If the source term (the applied given force on the medium) is time independent, and if we are given an arbitrarily coarse conforming mesh (triangulation in 2D, tetrahedrization in 3D), the proposed MHM method consists in first solving a series of fully decoupled (therefore parallelizable) local (element-wise) problems defining parts of the full solution variables which are directly related to the source term, followed by the solution of a global (coarse) problem, which yields the degrees of freedom of both the Lagrange multiplier dependent part of the full solution variables and the Lagrange multiplier itself. Finally, the updating of the full solution variables is obtained by adding each splitted solution variables, before going on the next time step of a leap-frog time integration scheme. Theoretical analysis and implementation of this MHM method where the local problems are discretized with a DG method, are underway.

6.3. High performance numerical computing

6.3.1. Poring a DGTD solver for bioelectromagnetics to the DEEP-ER architecture

Participants: Alejandro Duran [Barcelona Supercomputing Center, Spain], Stéphane Lanteri, Raphaël Léger, Damian A. Mallón [Juelich Supercomputing Center, Germany].

We are concerned here with the porting of the GERShWIN DGDT solver for computational bioelectromagnetics to the novel heterogeneous architecture proposed in the DEEP-ER european project on exascale computing. This architecture is based on a Cluster/Booster division concept (see Fig. 5). The Booster nodes are based on the Intel Many Integrated Core (MIC) architecture. Therfore, one objective of our efforts is the algorithmic adaptation of the DG kernels in order to leverage the vectorizing capabilities of the MIC processor. The other activities that are undertaken in the context of our contribution to this project aim at exploiting the software environments and tools proposed by DEEP-ER partners for implementing resiliency strategies and high performance I/O operations. In particular, the Cluster nodes are used for running some parts of the pre- and post-processing phases of the DGTD solver which do not lend themselves well to multithreading, as well as I/O intensive routines. One possibility to achieve this is to consider a model in which these less scalable and I/O phases are reverse-offloaded from Booster processes to Cluster processes in a one-to-one mapping. This is achieved by exploiting the OmpSs offload functionality, developed at Barcelona Supercomputing Center for the DEEP-ER platform.

6.3.2. High order HDG schemes and domain decomposition solvers for frequency-domain electromagnetics

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Matthieu Kuhn [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri, Ludovic Moya, Olivier Rouchon [CINES, Montpellier].

This work is undertaken in the context of the ANR TECSER project on one hand, and PRACE 4IP project on the other hand, and is concerned with the development of scalable frequency-domain electromagnetic wave propagation solvers, in the framework of the HORSE simulation software. HORSE is based on a high order HDG scheme formulated on an unstructured tetrahedral grid for the discretization of the system of three-dimensional Maxwell equations in heterogeneous media, leading to the formulation of large sparse undefinite linear system for the hybrid variable unknowns. This system is solved with domain decomposition strategies

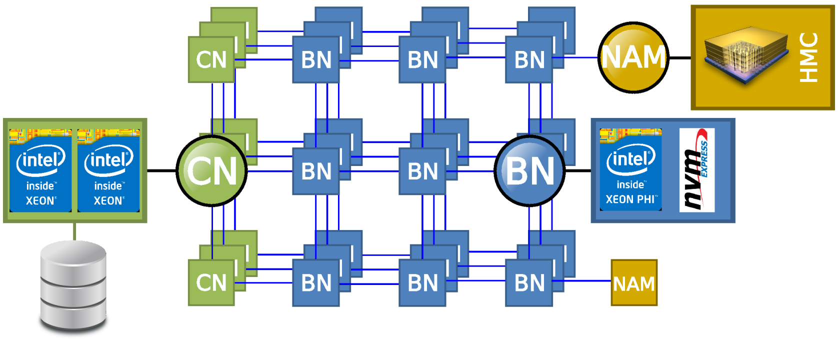


Figure 5. DEEP-ER hardware architecture sketch.

that can be either a purely algebraic algorithm working at the matrix operator level (i.e. a black-box solver), or a tailored algorithm designed at the continuous PDE level (i.e. a PDE-based solver). In the former case, we use the MaPHyS (Massively Parallel Hybrid Solver) developed in the HIEPACS project-team at Inria Bordeaux - Sud-Ouest.

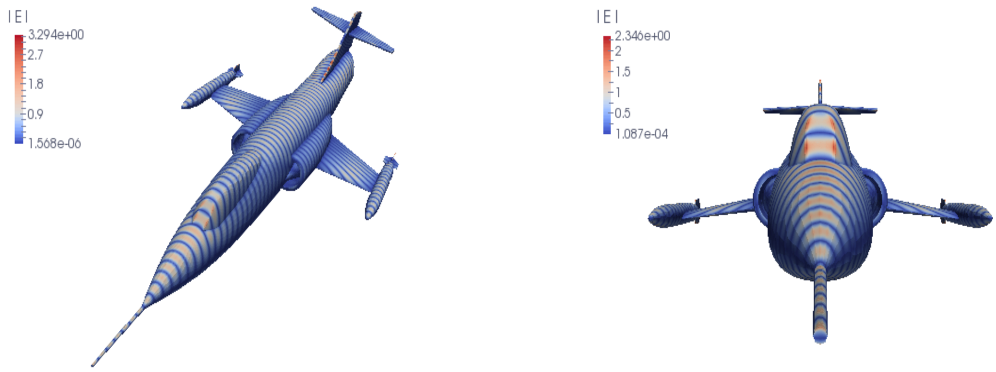


Figure 6. Scattering of a plane wave by a Lockheed F-104 Starfighter. Contour lines of the amplitude of the electric field. Simulations are performed with a HDG scheme based on a cubic interpolation of the electric and magnetic field unknowns, combined with a PDE-based domain decomposition solver.

6.4. Applications

6.4.1. Light diffusion in nanostructured optical fibers

Participants: Wilfried Blanc [Optical Fibers team, LPMC, Université Nice Sophia Antipolis, Nice], Stéphane Lanteri, Paul Loriot, Claire Scheid.

Optical fibers are the basis for applications that have grown considerably in recent years (telecommunications, sensors, fiber lasers, etc.). Despite these undeniable successes, it is necessary to develop new generations of amplifying optical fibers that will overcome some limitations typical of silica. In this sense, the amplifying

Transparent Glass Ceramics (TGC), and particularly the fibers based on this technology, open new perspectives that combine the mechanical and chemical properties of a glass host and the augmented spectroscopic properties of embedded nanoparticles, particularly rare earth-doped oxide nanoparticles. Such rare earth-doped silica-based optical fibers with transparent glass ceramic (TGC) core are fabricated by the Optical Fibers team of the Laboratory of Condensed Matter Physics (LPMC) in Nice. The objective of this collaboration with Wilfried Blanc at LPMC is the study of optical transmission terms of loss due to scattering through the numerical simulation of light propagation in a nanostructured optical fiber core using a high order DGTD method developed in the team.

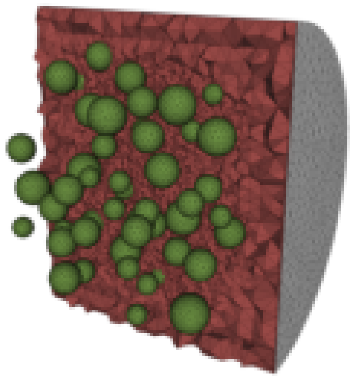


Figure 7. Unstructured tetrahdral mesh of a nanostructured optical fiber core.

6.4.2. Gap-plasmon confinement with gold nanocubes

Participants: Stéphane Lanteri, Antoine Moreau [Institut Pascal, Université Blaise Pascal], Claire Scheid, Jonathan Viquerat.

The propagation of light in a slit between metals is known to give rise to guided modes. When the slit is of nanometric size, plasmonic effects must be taken into account, since most of the mode propagates inside the metal. Indeed, light experiences an important slowing-down in the slit, the resulting mode being called *gap-plasmon*. Hence, a metallic structure presenting a nanometric slit can act as a light trap, i.e. light will accumulate in a reduced space and lead to very intense, localized fields. Recently, the chemical production of random arrangements of nanocubes on gold films at low cost was proved possible by Antoine Moreau and colleagues at Institut Pascal. Nanocubes are separated from the gold substrate by a dielectric spacer of variable thickness, thus forming a narrow slit under the cube. When excited from above, this configuration is able to support gap-plasmon modes which, once trapped, will keep bouncing back and forth inside the cavity. At visible frequencies, the lossy behavior of metals will cause the progressive absorption of the trapped electromagnetic field, turning the metallic nanocubes into efficient absorbers. The frequencies at which this absorption occurs can be tuned by adjusting the dimensions of the nanocube and the spacer. In collaboration with Antoine Moreau, we propose to study numerically the impact of the geometric parameters of the problem on the behaviour of a single nanocube placed over a metallic slab (see Fig. 8). The behavior of single nanocubes on metallic plates has been simulated, for lateral sizes c ranging from 50 to 80 nm, and spacer thicknesses δ from 3 to 22 nm. The absorption efficiency in the cube Q_{cube} at the resonance frequency is retrieved from the results of each computation (see Fig. 9).

6.4.3. Dielectric reflectarrays

Participants: Maciej Klemm [Centre for Communications Research, University of Bristol], Stéphane Lanteri, Claire Scheid, Jonathan Viquerat.

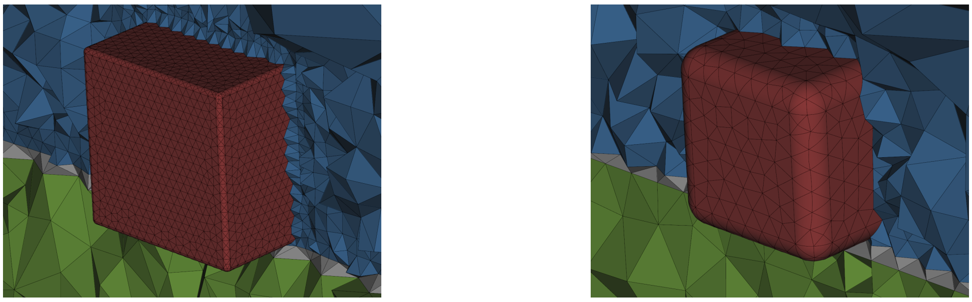
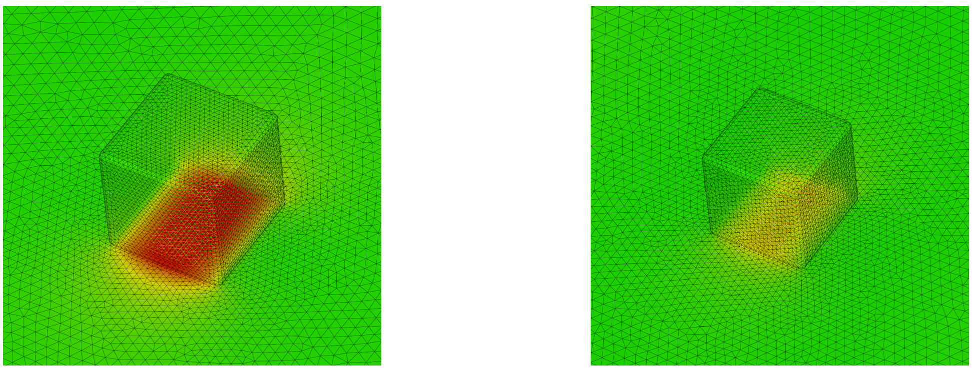


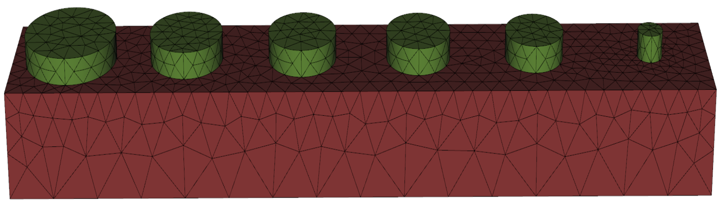
Figure 8. Meshes of rounded nanocubes with rounding radii ranging from 2 to 10 nm. Red cells correspond to the cube. The latter lies on the dielectric spacer (gray cells) and the metallic plate (green). Blue cells represent the air surrounding the device.



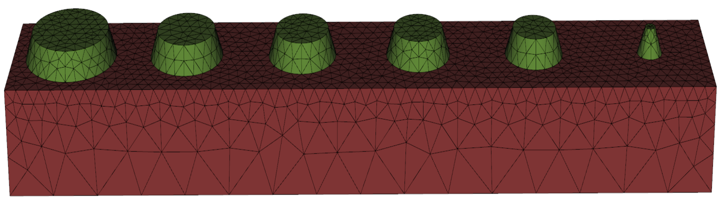
$c = 70$ nm, $\delta = 12$ nm $\qquad$ $c = 60$ nm, $\delta = 18$ nm

Figure 9. Amplitude of the discrete Fourier transform of the magnetic field for different nanocube configurations. All field maps are scaled identically for better comparison. The obtained field is more intense for configurations that yield high Q_{cube} values.

In the past few years, important efforts have been deployed to find alternatives to on-chip, low-performance metal interconnects between devices. Because of the ever-increasing density of integrated components, intra- and inter-chip data communications have become a major bottleneck in the improvement of information processing. Given the compactness and the simple implantation of the devices, communications *via* free-space optics between nanoantenna-based arrays have recently drawn more attention. Here, we focus on a specific low-loss design of dielectric reflectarray (DRA), whose geometry is based on a periodic repartition of dielectric cylinders on a metallic plate. When illuminated in normal incidence, specific patterns of such resonators provide a constant phase gradient along the dielectric/metal interface, thus altering the phase of the incident wavefront. The gradient of phase shift generates an effective wavevector along the interface, which is able to deflect light from specular reflection. However, the flaws of the lithographic production process can lead to discrepancies between the ideal device and the actual resonator array. Here, we propose to exploit our DGTD solver to study the impact of the lithographic flaws on the performance of a 1D reflectarray (see Fig. 10). Efficient computations are obtained by combining high-order polynomial approximation with curvilinear meshing of the resonators, yielding accurate results on very coarse meshes (see Fig. 11). The study is continued with the computation of the reflection of a 2D reflectarray. This work constitutes the base of a wider study in collaboration with Maciej Klemm at the Centre for Communications Research, University of Bristol.

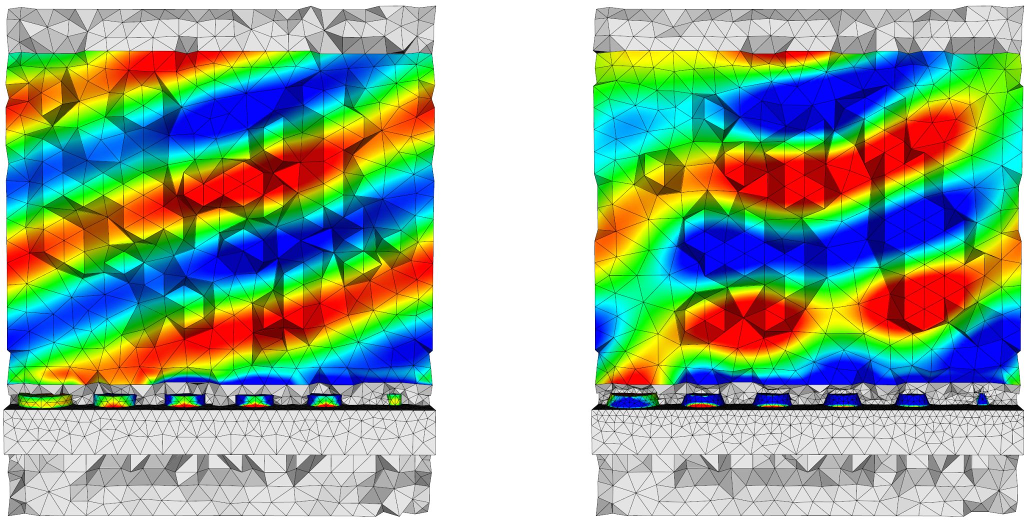


Ideal reflectarray



Realistic reflectarray

Figure 10. Ideal and realistic 1D dielectric reflectarray meshes. The red tetrahedra correspond to silver, while the green ones are made of an anisotropic dielectric material. The device is surrounded by air and terminated by a PML above and below, and by periodic boundary conditions on the lateral sides.



Ideal reflectarray — Realistic reflectarray

Figure 11. Time-domain snapshot of E_y component for ideal and realistic 1D dielectric reflectarrays. Solution is obtained in established regime at $t = 0.1$ ps. Fields are scaled to $[-1, 1]$.

NANO-D Project-Team

6. New Results

6.1. Development of a novel minimization method

Participants: Clement Beitone, Stephane Redon.

Finding the optimized configuration of a system of particles so that it minimizes the energy of the system is a very common task in the field of particles simulation. More precisely, we are interested in finding the closest atomic structure located at a minima on the Potential Energy Surface (PES) starting from a given initial configuration. Achieving faster but reliable minimizations of such systems help to enhance a wide range of applications in molecular dynamics. To improve the efficiency of the convergence some authors have proposed alternative methods to the steepest descent algorithm; for example, the conjugate gradient technique or the Fast Inertial Relaxation Engine (FIRE).

In this work, we are developing a novel method that helps to increase the efficiency and the reliability of existing optimizers, *e.g.* FIRE and Interactive Modelling (IM).

We have implemented the modified versions of these algorithms along with others optimization algorithms like L-BFGS and Conjugate Gradient as state updaters in SAMSON. To assess the efficiency of the proposed approaches we have developed an App in SAMSON that allows us to reliably and conveniently probe several criteria during the minimization process (Figure 3).

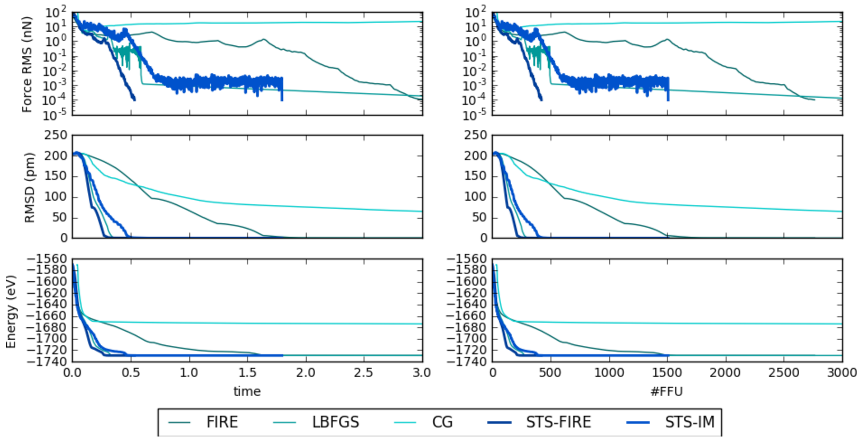


Figure 3. Comparison of different optimizers with the proposed methods on the fullerene C240. For this experiment the force field used to model the interactions between the atoms is the Brenner potential.

6.2. Parallel algorithms for adaptive molecular dynamics simulations

Participants: Dmitriy Marin, Stephane Redon.

We have developed a parallel implementation of Adaptively Restrained Particle Simulations (ARPS) in LAMMPS Molecular Dynamics Simulator with the usage of Kokkos [0] package. The main idea of the ARPS method [22] is to speed up particle simulations by adaptively switching on and off positional degrees of freedom, while letting momenta evolve; this is done by using adaptively restrained Hamiltonian. The developed parallel implementation allows us to run LAMMPS with ARPS integrator on central processing units (CPU), graphics processing units (GPU), or many integrated core architecture (MIC). We modified the ARPS algorithm for efficient usage of GPU and many-core CPU, e.g. all computations were parallelized for efficient calculations on computational device; communications between host and device were decreased.

To measure speed up of the developed parallel implementation we used several benchmarks and heterogeneous computational systems with next parameters: 2x CPU Intel Xeon E5-2680 v3 (24 cores in total), GPU Nvidia Quadro K4200, GPU Nvidia Tesla K20c. Results on the speed up in comparison with serial ARPS code for one of the benchmarks (Lennard–Jones liquid, 515K atoms, ∼1% of particles switches their state at each timestep from active to restrained or from restrained to active) are shown in Figure 4 . It can be seen, that for small number of CPU cores the speed up is almost constant for all the percentage of active atoms in the system. But for large number of CPU cores and for GPUs the speed up is decreasing with decreasing percentage of active atoms, because of divergence of threads and limited occupancy. The achieved speed up on 20 CPU-cores is up to 14 times, on GPU Nvidia Tesla K20c is up to 24 times.

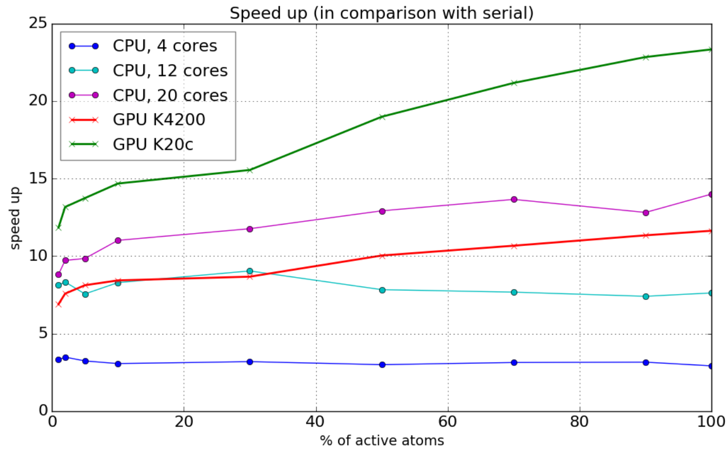


Figure 4. The parallel ARPS results

6.3. Adaptive Algorithms for Orbital-Free Density Functional Theory

Participants: Francois Rousse, Stephane Redon.

The SAMSON App developed to simulate molecular systems with an adaptive version of OF-DFT has been continued. It has been tested on several small systems : atoms, dimers, etc. The errors found on the energies and the bond length found were coherent with the predictive characteristics of OF-DFT and with other OF-DFT softwares like PROFESS.

[0] The Kokkos package is based on Kokkos library, which is a templated C++ library that provides two key abstractions: it allows a single implementation of an application kernel to run efficiently on different hardware, such as a many-core CPU, GPU, or MIC; it provides data abstractions to adjust (at compile time) the memory layout of basic data structures — like 2d and 3d arrays — for performance optimization on different platforms. These abstractions are set at build time (during compilation of LAMMPS).

The pseudopotentials computed by the Carter Group of Princeton (who developed PROFESS) have been implemented in the SAMSON App. The electronic densities became smoother and the predictions were improved, but it restricted the applicability of the SAMSON App since the pseudopotentials were computed only for the elements of the columns III (like aluminum) and V (like Potassium) of the periodic table.

Several optimization algorithms have been tried : projected gradient, Primal-Dual, Lagrangian multiplier improved with a penalization, different nonlinear conjugate gradient minimization algorithms ... None of them showed a clear superiority on the other in both stability and speed. Currently, we use the projected gradient since it is the most stable.

We have implemented an interaction model in SAMSON based on the OF-DFT code and tested its ability to predict the geometry of system on a small crystal of aluminum. The crystal contracted itself, which is coherent with the OF-DFT theory, since it tends to underestimate bond lengths, and with the surface tension, since it tends to minimize the surface of the system. The next step will be to make this interaction model adaptive and measure how much time is gained.

6.4. A crystal creator app

Participants: Francois Rousse, Stephane Redon.

We developed a new SAMSON Element able to generate models of crystals. The user can either write its own unit cell or load it from a CIF file ("Crystallographic Information File"). Once written or imported, this unit cell can be replicated again in every direction to generate a whole crystal. As the important characteristics of crystals often comes from the defects, the replacements and the insertions, these repetitions of unit cells are not mere copies but are whole new unit cells generated again each time. Thus a crystal with enough unit cells shall have the right proportion of elements, with the right amount of defects, replacements and insertions, randomly disposed. In the document view, the unit cells are separated to ease the manipulation of the crystal. Last, it allows the user to cut the crystal on the planes given by Miller indexes.

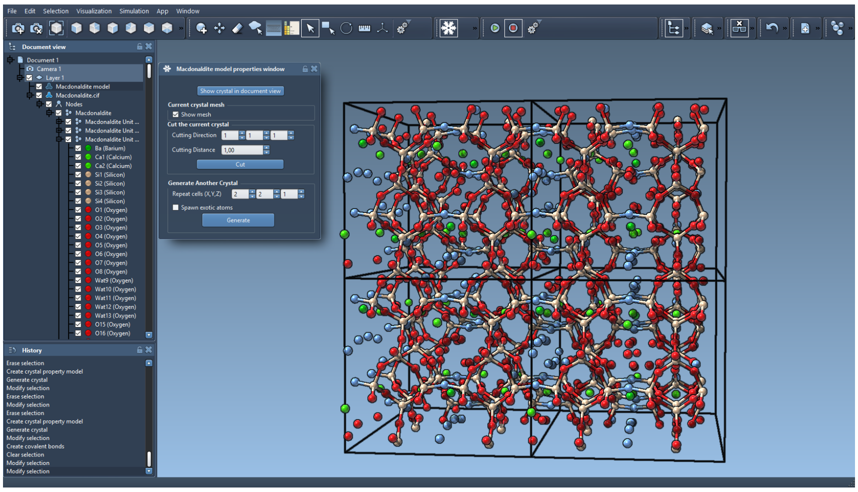


Figure 5. A Macdonaldite crystal generated in SAMSON

6.5. Software development process improvements

Participants: Jocelyn Gate, Stephane Redon.

We set up a Jenkins server on a virtual machine at Inria. The server is accessible to the team and is able to build and generate everything related to SAMSON. This Jenkins server is linked to diferents slaves, located in our offices:

- Window 7 / Windows 10
- Fedora 21 / Fedora 25 / Ubuntu 16.04
- MacOs 10.10.5

Slave machines are used by the Jenkins server to build the specified version of SAMSON, generate the associated SDK, build all SAMSON elements that are specified on Jenkins and upload everything to our private version of SAMSON Connect. Thanks to this, the team has access each day to the latest developments.

In order to efficiently upload everything from slaves nodes, Jenkins uses a private helpers that is able to communicate with SAMSON-Connect, and that knows every SAMSON files format.

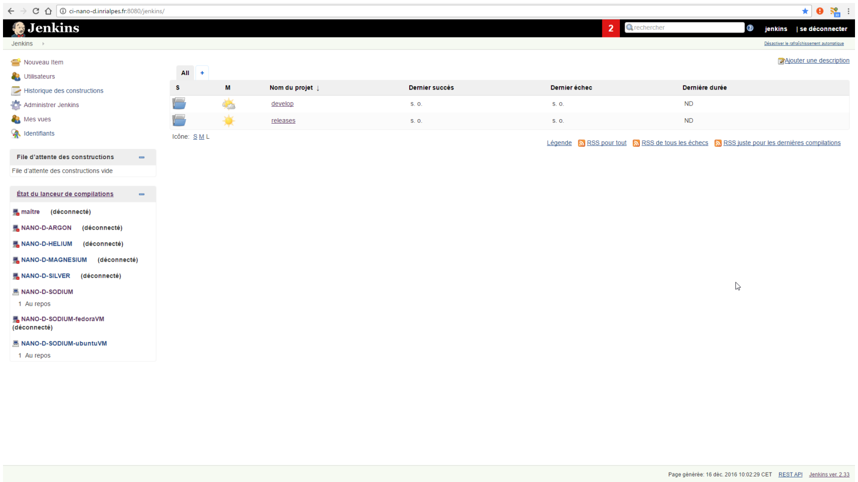


Figure 6. The jenkins interface

We developed a private, command line SAMSON helper that is able to do everything concerning the packing and the uploading of new versions of SAMSON, the SAMSON SDK and the installer to SAMSON Connect. It can:

- Upload the SAMSON or SAMSON-SDK packaged file to SAMSON-Connect (adding a new version of SAMSON/SAMSON-SDK).
- Upload the SAMSON or SAMSON-SDK Setup executable to SAMSON-Connect.
- Package the SAMSON elements of a developer to .element files.
- Upload .element files to SAMSON Connect.

6.6. Updates to SAMSON and SAMSON Connect

Participants: Jocelyn Gate, Stephane Redon.

To be able to know if SAMSON works well on users computers, we added some logging features inside SAMSON, SAMSON installers and SAMSON Helpers. Thanks to this functionality, users may accept to send logs when bugs are found. For example, if SAMSON crashes on a user computer, a log is generated, anonymized, and automatically sent to the SAMSON Connect web service. If SAMSON crashes because of a SAMSON Element, an email is sent to the author of the SAMSON Element. If a new user tries to install SAMSON or the SAMSON SDK, a log is sent to the SAMSON Connect web service.

We also added the possibility for users to configure proxy access to SAMSON Connect. These functionalities will be part of the upcoming 0.6.0 release of SAMSON.

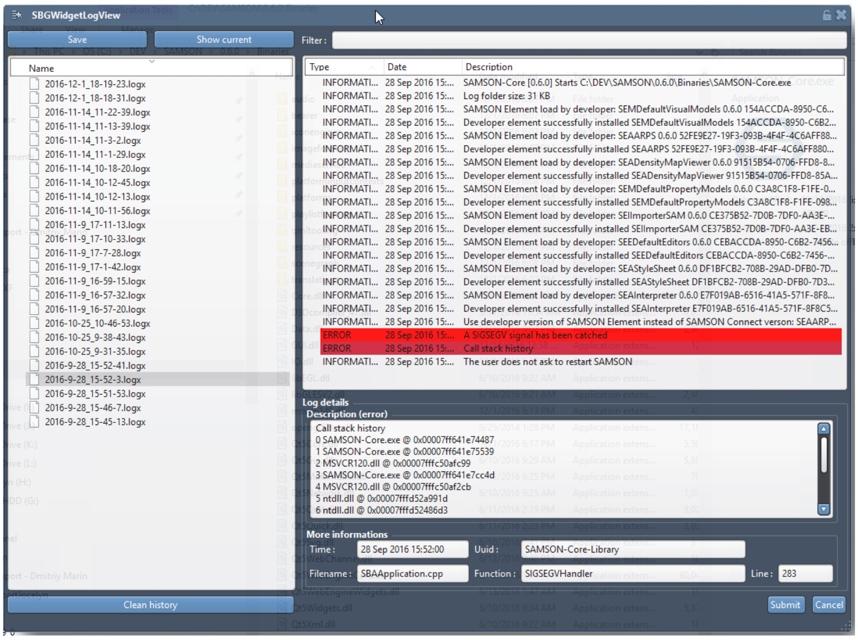


Figure 7. The SAMSON log interface

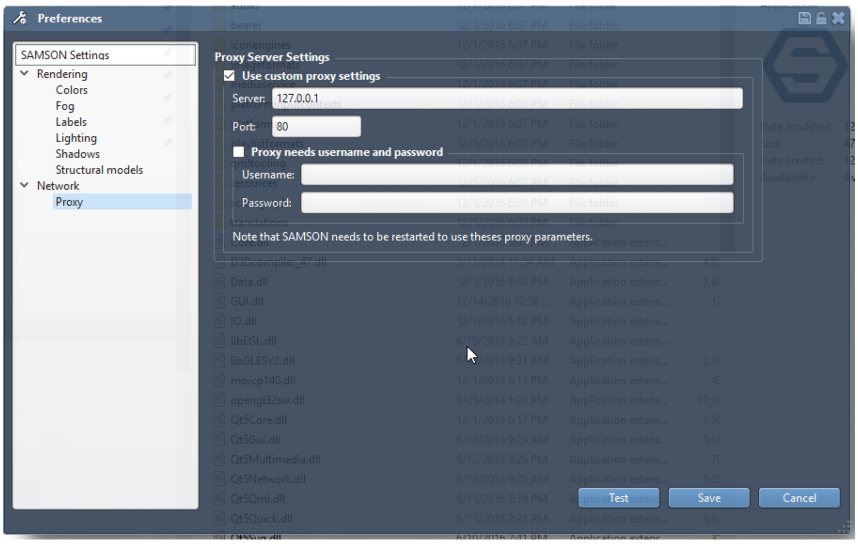


Figure 8. The proxy setting interface

6.7. As-Rigid-As-Possible molecular interpolation paths

Participants: Minh Khoa Nguyen, Leonard Jaillet, Stephane Redon.

We submitted a paper describing a new method to generate interpolation paths between two given molecular conformations. It applies the As-Rigid-As-Possible (ARAP) from the field of computer graphics to manipulate complex meshes while preserving their essential structural characteristics. The adaptation of ARAP interpolation approach to the case of molecular systems was presented. Experiments were conducted on a large set of benchmarks and the performance was compared between ARAP interpolation and linear interpolation. They show that ARAP interpolation generates more relevant paths, that preserve bond lengths and bond angles better.

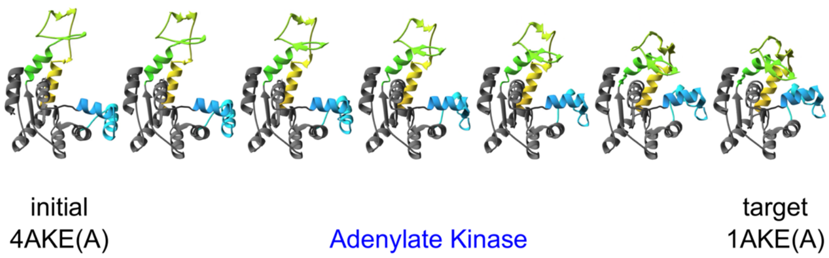


Figure 9. The morphing path for Adenylate Kinase from 4AKE (chain A) to 1AKE (chain A) by ARAP interpolation:

6.8. As-Rigid-As-Possible molecular interpolation paths

Participants: Krishna Kant Singh, Stephane Redon.

We have continued our work on the development of parallel adaptively restrained particle simulations. We proposed new algorithms to compute forces involving active particles faster. These algorithms involved construction of the Active Neighbor List (ANL) and incremental force computations. These algorithms have advantages over the state-of-the-art methods for simulating a system using Adaptively Restrained Molecular Dynamics (ARMD). Previously proposed algorithms required at-least 60% restrained particles in order to achieve speed up. In new algorithms, we overcome this limitation and speed up can be achieve with 10% retrained particles. We implemented our algorithm in the popular molecular dynamics package LAMMPS and submitted our results in the *Computer Physics Communications* Journal [0]. Figure 11 show that speed-up can be achieved for more than 10% of the particles are restrained. We also achieved significant speed up in constructing the ANL (figure 12).

6.9. Refining the energy landscape sampling of protein-protein associations

Participants: Dmytro Kozakov, Leonard Jaillet.

PIPER is a FFT-based protein docking program with pairwise potentials. It combines a systematic sampling procedure with an original pairwise potential that provides an energy landscape representation through a set of samples [48].

[0] K.K. Singh, S. Redon, Adaptively Restrained Molecular Dynamics in LAMMPS, Submitted to *Computer Physics Communications*.

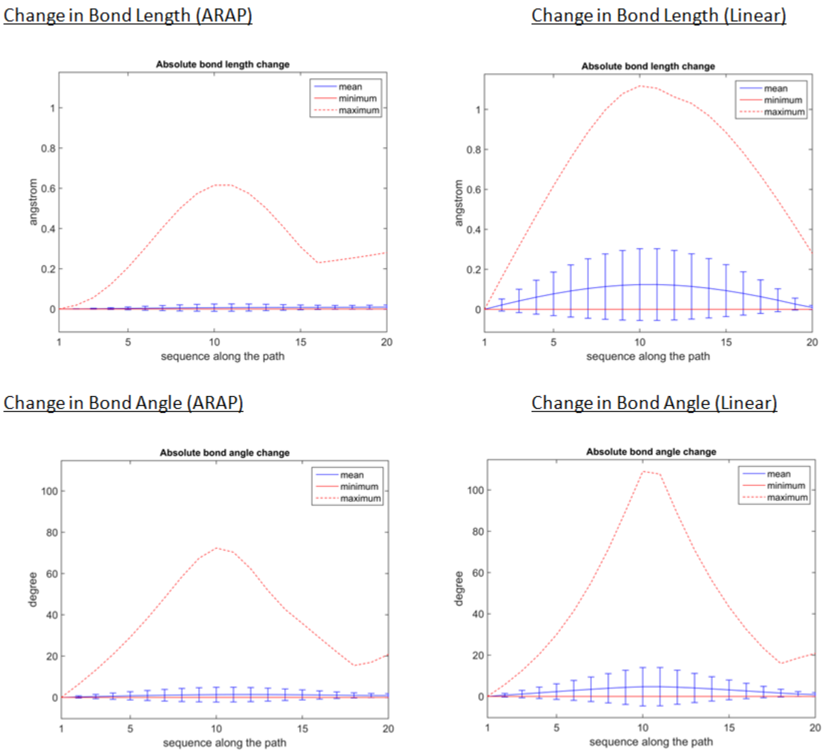


Figure 10. Comparison of ARAP and linear interpolation for preserving structural characteristics of adenylate kinase

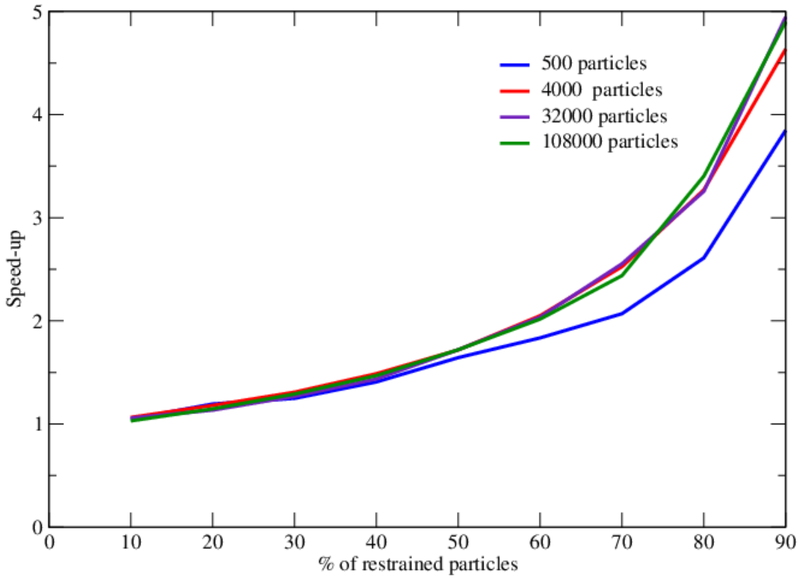


Figure 11. speed up using ARMD on different benchmark

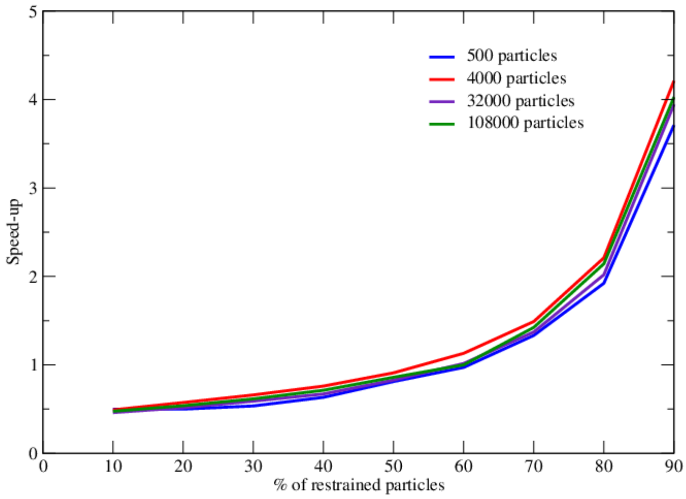


Figure 12. Obtained speed up in constructing the ANL.

In [49], an experimental validation of the complexes obtained with PIPER, has been made possible thanks to the PRE method [31]. PRE (NMR paramagnetic relaxation enhancement) is an experimental technique used to characterize the states present for a given system. Hence, it characterizes the accessible region of the energy landscape corresponding to a given protein. For this, it introduces paramagnetic labels (tags) one at a time at few sites on one protein. The method then relies on measures of the transverse paramagnetic relaxation enhancement rates of the backbone amide protons (HN) of the partner protein. These value correspond to the weighted averages of the values for the various states present. One advantage of PRE is that it is nicely sensitive to lowly populated states.

In [49] the values measured obtained from a set of PIPER output have been compared to those obtained when using only the native state. It appears that using all the PIPER states give a better correlation respect to experimental results than when using only the native state.

In this context, our objective is to refine the energy landscape description by filtering some of the PIPER output complexes in order to improve even further the correlation with experimental measures. The method is developed as a module of the SAMSON software package (http://www.samson-connect.net/).

We have proposed a refinement from process of PIPER complexes based on two criterions: a RMSD-based filtering and an energy-based filtering.

The RMSD-filtering first creates a graph of connected component by connecting a pair of complexes if their distance is lower than a given RMSD threshold. Such a process forms clusters. Then, only the complexes that are in the cluster where belongs the native state are conserved. Since only rigid transforms are applied, RMSD are computed thanks to the fast RMSD computation method previously proposed in the team [56].

The energy-based filtering compares the energy of the complexes to the native state energy. The states for which the difference of energy is higher than a given threshold are discarded.

We have evaluated the results obtained when using our filtering scheme, for a distance threshold ranging form 3 to 9 and for an energy threshold ranging from 70 to $240 kJ.mol^{-1}$. Some setting of the filtering are able to improve the correlation (see figure 13), but the gain around 0.3% remains limited (e.g. the correlation rising from 0.770 to 0.773). We are currently working on a more sophisticated state selection process to filter more precisely the PIPER states and hence to further improve the correlation.

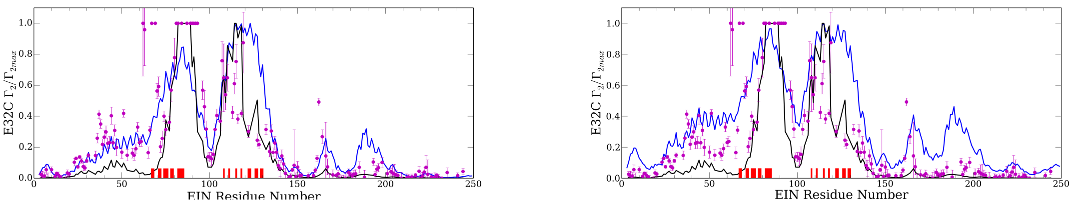


Figure 13. The experimental PRE rates ($\Gamma 2$) are displayed as filled-in magenta circles. Theoretical intermolecular PREs, calculated only from the coordinates of the specific EIN/HPr complex, are shown as black lines. Calculated PRE values from PIPER output are shown as blue lines. The calculated PRE value obtained from the filtered complexes (left) gives a higher correlation with experimental ($c = 0.773$) than the correlation obtained from all the complexes generated with PIPER (right) ($c = 0.770$).

6.10. CREST: Chemical Reactivity Exploration with Stochastic Trees

Participants: Leonard Jaillet, Stephane Redon.

We have proposed the CREST method (Chemical Reactivity Exploration with Stochastic Trees), a new simulation tool to assess the chemical reaction paths of molecular systems. First, it builds stochastic trees based on motion planning principles to search for relevant pathways inside a system's state space. This generates low energy paths transforming a reactant to a given product. Then, a nudged elastic band optimization step locally improves the quality of the initial solutions. The consistency of our approach has been evaluated through tests in various scenarios. It shows that CREST allows to appropriately describe conformational changes as well as covalent bond breaking and formations present in chemical reactions (see figure 14).

This contribution appears in continuity of our previous work regarding the development of a geenric Motion planning architecture for nanosystems. Important features have been added to specifically treat the case of chemical reaction, such as structure alignment, exploration based on multiple trees, automatic resizing of the sampling volume, etc.

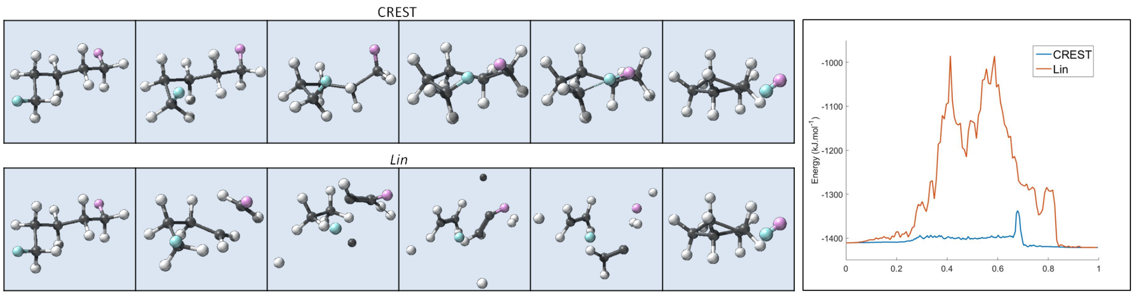


Figure 14. Fictive chemical reaction transforming a pentane into a cyclopentane with a H2 molecule. Hydrogen atoms leading to the H2 molecule are colored. The path obtained with CREST (top) is able to capture the CH3 internal rotations that approaches the two H2 Hydrogens and thus, lead to a low energy barrier. By comparison, a method based on linear interpolation (Lin) gives intermediate broken structures after local path optimization (down). The plot on the right shows the respective energies along the paths. This represents Scenario 3 described in our Results section.

6.11. IM-UFF: extending the Universal Force Field for interactive molecular modeling

Participants: Leonard Jaillet, Svetlana Artemova, Stephane Redon.

We have completed the development of IM-UFF (Interactive Modeling - UFF), an extension of UFF that combines the possibility to significantly modify molecular structures (as with reactive force fields) with a broad diversity of supported systems thanks to the universality of UFF. Such an extension lets the user easily build and edit molecular systems interactively while being guided by physically-based inter-atomic forces. This approach introduces weighted atom types and weighted bonds, used to update topologies and atom parameterizations at every time step of a simulation. IM-UFF has been evaluated on a large set of benchmarks and is proposed as a self-contained implementation integrated in a new module for the SAMSON software platform for computational nanoscience.

This contribution has been submitted to the Journal of Molecular Modeling.

6.12. Incremental methods for long range interactions

Participants: Semeho Edorh, Stephane Redon.

Adaptively Restrained Particles Simulations (**ARPS**) were recently proposed with the purpose of speeding up molecular simulations. The main idea is to modify the Hamiltonian such that the kinetic energy is set to zero for low velocities, which allows to save computational time since particles do not move and forces need not be updated.

We continued our work on developing an extension of **ARPS** to electrostatic simulations.

We have decided to compute the electrostatic contribution by using Multigrid method. This choice have been made because of its $\mathcal{O}(N)$ behavior and its good scalability. In systems containing point charges, Multigrid can't be applied directly because of the discontinuous distribution created by these charges. To overcome this problem, one can replace this distribution by a smooth charge distribution. This charge distribution will be the source term of a Poisson equation which will be solved by Multigrid method. By doing so we retrieve an approximative electrostatic contribution which can be corrected by a near field correction. Concretely each charge will be smeared by a smooth density function.This function is chosen with a compact support. The accuracy of the method is related to the degree of smoothness and the size of the support r_{cut} of the chosen function Fig(15). The bottleneck of this method is often the time spent building the smooth charge distribution. To overcome this issue, We've introduced an interpolation scheme in the near field correction. This leads to a significant reduction of the support required to achieve a specified accuracy. The time spent building the smooth charge distribution is also reduced. Conversely the near correction is slowed down. Nevertheless, the introduction of the interpolation scheme speeds up the method in most of cases Fig(16).

Finally we modified our algorithm to take advantage of ARPS dynamics. This leads to a speed up related to the amount of restrained particles. According to our benchmarks our method can challenge Particle Particle Particle Mesh(**PPPM**), the traditional fast method to compute electrostatics Fig(17). Our algorithm is implemented in LAMMPS.

6.13. Error Analysis of Modified Langevin Dynamics

Participants: Zofia Trstanova, Gabriel Stoltz, Stephane Redon.

We performed a mathematical analysis of modified Langevin dynamics. The aim of this work was first to prove the ergodicity of the modified Langevin dynamics (which fails to be hypoelliptic), and next to analyze how the asymptotic variance on ergodic averages depends on the parameters of the modified kinetic energy. Numerical results illustrated the approach, both for low-dimensional systems where we resorted to a Galerkin approximation of the generator, and for more realistic systems using Monte Carlo simulations.

6.14. Estimating the speed-up of Adaptively Restrained Langevin Dynamics

Participants: Zofia Trstanova, Stephane Redon.

We performed a computational analysis of Adaptively Restrained Langevin dynamics, in which the kinetic energy function vanishes for small velocities. Properly parameterized, this dynamics makes it possible to reduce the computational complexity of updating inter-particle forces, and to accelerate the computation of ergodic averages of molecular simulations. We analyzed the influence of the method parameters on the total achievable speed-up. In particular, we estimated both the algorithmic speed-up, resulting from incremental force updates, and the influence of the change of the dynamics on the asymptotic variance. This allowed us to propose a practical strategy for the parametrization of the method. We validated these theoretical results by representative numerical experiments on the system of a dimer surrounded by a solvent.

6.15. Stable and accurate schemes for Langevin dynamics with general kinetic energies

Participants: Zofia Trstanova, Gabriel Stoltz.

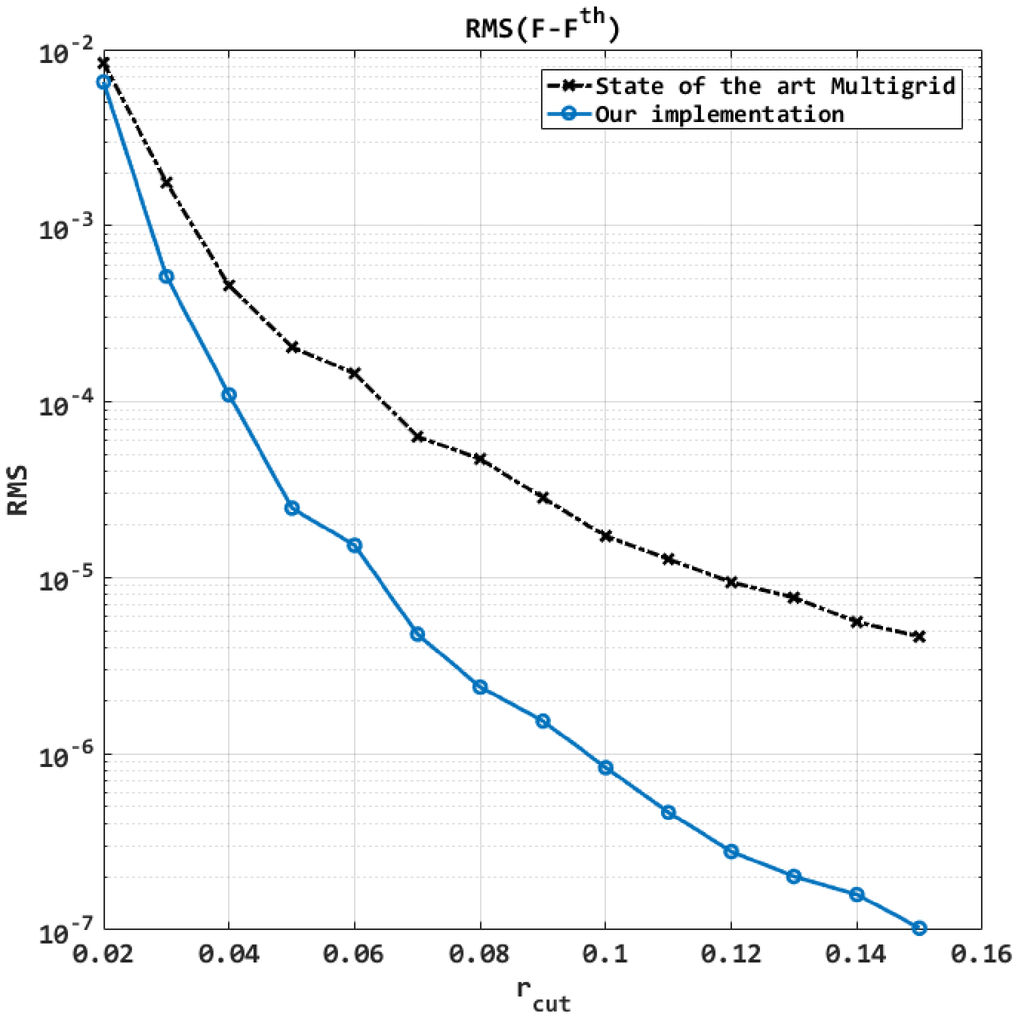


Figure 15. Accuracy in forces for the state of the art multigrid and our implementation : 125000 charged particles randomly distributed in a cubic box. r_{cut} represents the width of the chosen function.

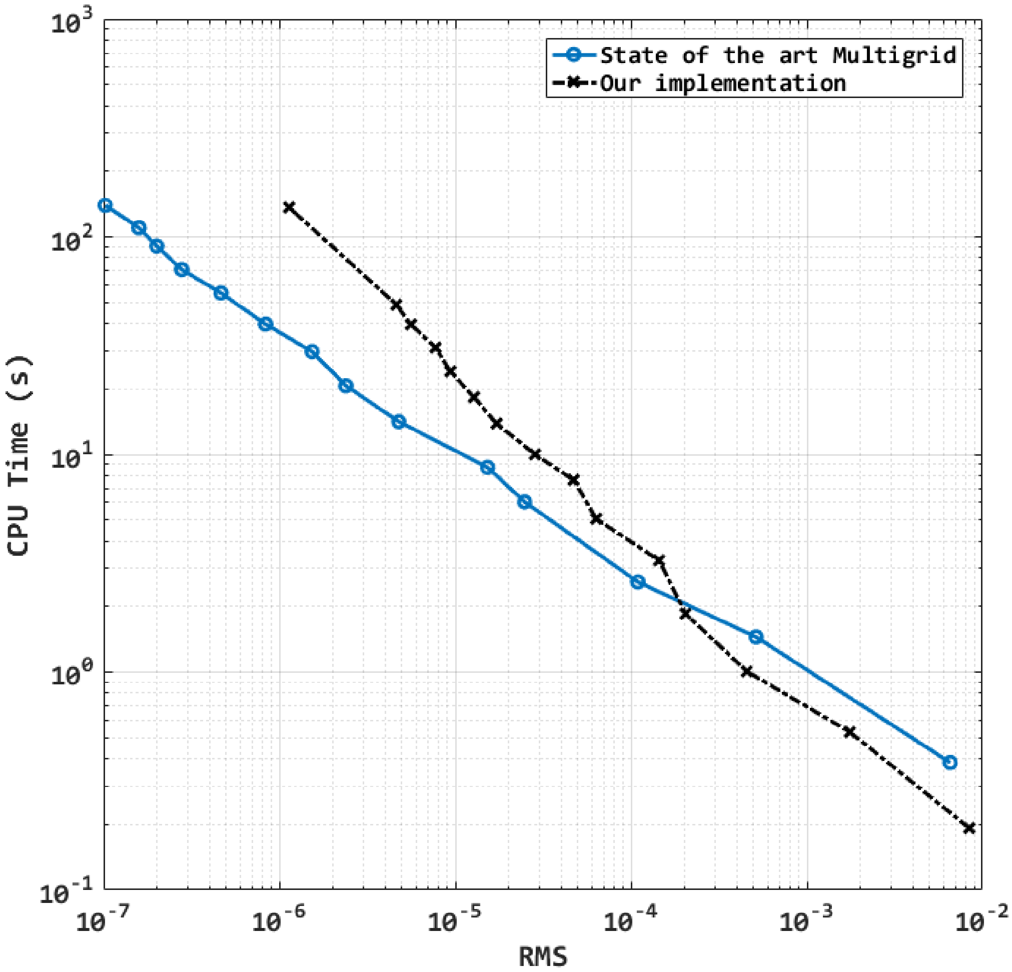


Figure 16. Comparison in terms of CPU time between the state of the art multigrid and our implementation : 125000 charged particles randomly distributed in a cubic box. r_{cut} represents the width of the chosen function.

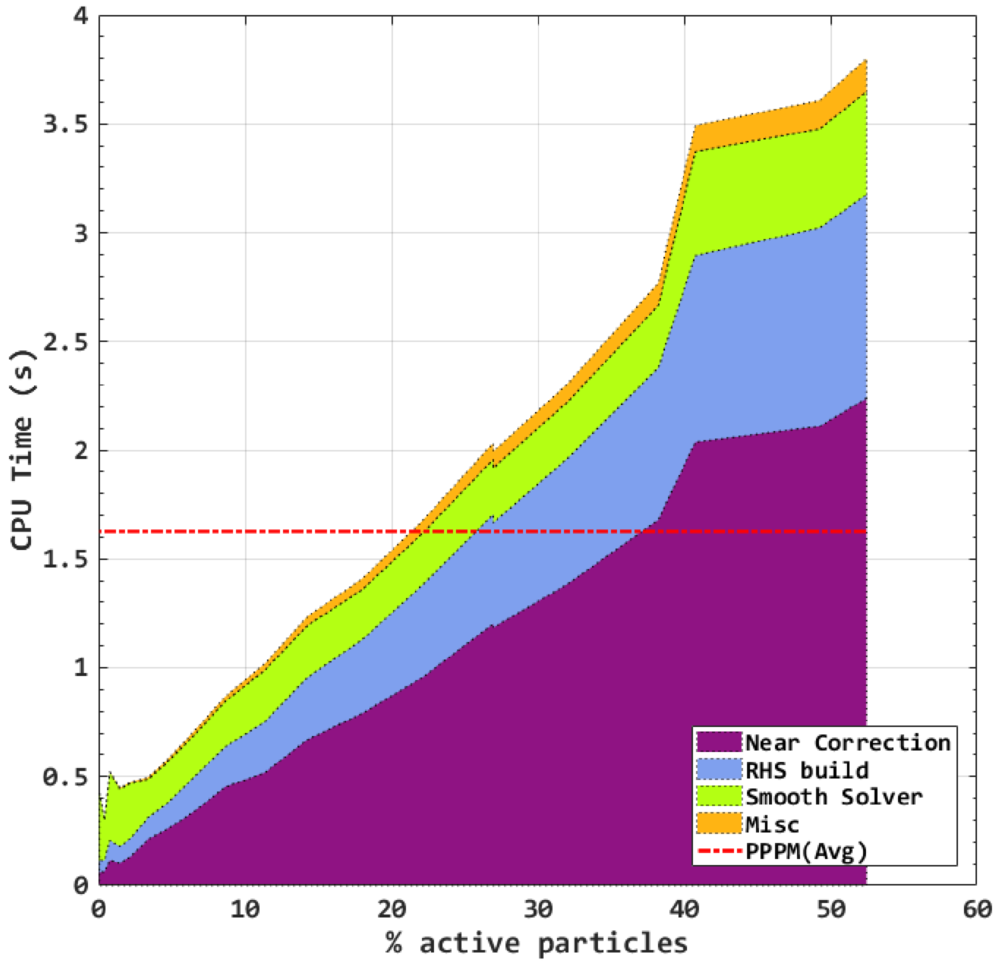


Figure 17. Comparison in terms of CPU time between PPPM and our implementation for a fixed accuracy : 64000 charged particles randomly distributed in a cubic box. Some particles are in restrained dynamics. Colored areas show the associated contribution of each part of our multigrid algorithm. Red dash-dot line represents CPU Time of Particle Particle Particle Mesh needed for this system.

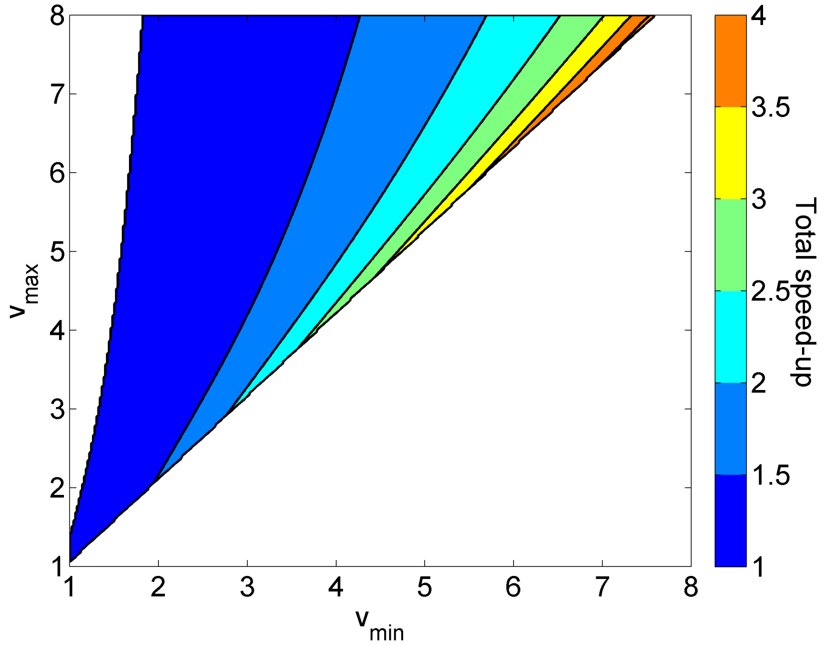


Figure 18. Analytical estimation of the total speed-up of the 3D simulation of the dimer in solvent. Only the solvent particles are restrained by the AR-method. We estimated the expected total speed-up S_{total} for the observable dimer distance A_D with respect to the restraining parameters $v_{\min}$ and $v_{\max}$ ($v_{\max} \leq 0.95 v_{\max}$). The variance was estimated from three points as a linear function of $v_{\min}$ and $v_{\max}$ and we used the analytical estimation of the algorithmic speed-up S_{a}. Only $S_{\text{total}} > 1$ is plotted.

We studied integration schemes for Langevin dynamics with a kinetic energy different from the standard, quadratic one in order to accelerate the sampling of the Boltzmann–Gibbs distribution. We considered two cases: kinetic energies which are local perturbations of the standard kinetic energy around the origin, where they vanish (this corresponds to the so-called adaptively restrained Langevin dynamics); and more general non-globally Lipschitz energies. We developed numerical schemes which are stable and of weak order two, by considering splitting strategies where the discretizations of the fluctuation/dissipation are corrected by a Metropolis procedure. We used the newly developed schemes for two applications: optimizing the shape of the kinetic energy for the adaptively restrained Langevin dynamics, and reducing the metastability of some toy models with non-globally Lipschitz kinetic energies.

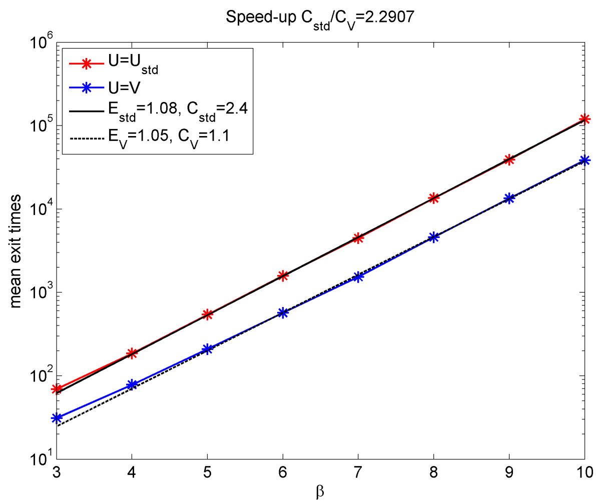


Figure 19. Comparison of the mean exit times for 2D double-well potential with the standard and the modified kinetic energy function (2000 realizations) as a function of the inverse temperature $\beta \in \{3, 4, 5, 6, 7, 8, 9, 10\}$. Thanks to the modified kinetic energy, the transition between two metastable states occurs on average three times faster.

6.16. Quadratic Programming Approach to Fit Protein Complexes into Electron Density Maps

Participants: Alexander Katrutsa, Sergei Grudinin.

We investigated the problem of simultaneous fitting protein complexes into electron density maps of their assemblies. These are represented by high-resolution cryo-EM density maps converted into overlapping matrices and partly show a structure of a complex. The general purpose is to define positions of all proteins inside it. This problem is known to be NP-hard, since it lays in the field of combinatorial optimization over a set of discrete states of the complex. We introduced quadratic programming approaches to the problem. To find an approximate solution, we converted a density map into an overlapping matrix, which is generally indefinite. Since the matrix is indefinite, the optimization problem for the corresponding quadratic form is non-convex. To treat non-convexity of the optimization problem, we use different convex relaxations to find which set of proteins minimizes the quadratic form best.

6.17. Inverse Protein Folding Problem via Quadratic Programming

Participants: Mikhail Karasikov, Sergei Grudinin.

We presented a method of reconstruction a primary structure of a protein that folds into a given geometrical shape. This method predicts the primary structure of a protein and restores its linear sequence of amino acids in the polypeptide chain using the tertiary structure of a molecule. Unknown amino acids are determined according to the principle of energy minimization. This study represents inverse folding problem as a quadratic optimization problem and uses different relaxation techniques to reduce it to the problem of convex optimizations. Computational experiment compares the quality of these approaches on real protein structures.

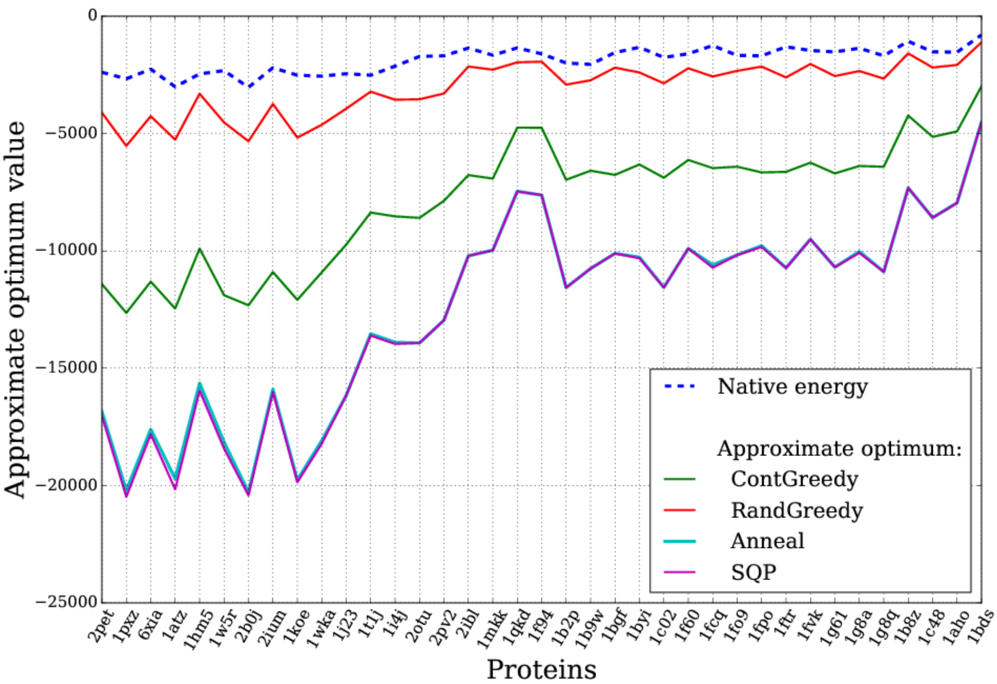


Figure 20. Approximate energy optimum for different relaxations computed on the test set

6.18. Coarse-Grained Protein Scoring Based on Geometrical Features

Participants: Mikhail Karasikov, Sergei Grudinin.

We learnt a scoring function to score protein structures with application to highly important problems in structural biology, namely, protein design, side-chain prediction, and selection of mutations increasing protein stability. For each native structure P_0 a set of ordered decoy structures $\mathcal{D}$ is given:

$$\mathcal{D} = \{P_1, \cdots, P_m\} \subset \mathcal{P},$$

$$(i_1, \cdots, i_m): \ P_{i_m} \preceq \cdots \preceq P_{i_1} \prec P_0.$$

The problem is to train protein scoring function

$$S : \mathcal{P} \to \mathbb{R},$$

such that

$$S(P_0) < S(P_{i_1}) \leq \cdots \leq S(P_{i_m}).$$

We proposed a residue-based scoring function, which uses not the positions of protein's atoms separately, but configurations of the entire residues. The proposed method requires artificially generated decoy structures for the training process and provides high quality scoring functions, which are efficient to compute. Several types of scoring functions are considered according to restrictions imposed by the specific application. For the prediction problems where the whole domain should be searched for the best prediction, we use functions that allow the reduction of emerging optimization problem

$$\sum_{k=1}^{m} \sum_{l=1}^{m} E_{kl}(a_k, a_l) \to \min_{(a_1,\cdots,a_m)\in\mathcal{A}^m} \tag{6}$$

to quadratic binary constrained optimization

$$\begin{aligned} &\underset{\vec{x}\in\{0,1\}^n}{\text{minimize}} && \vec{x}^{\mathsf{T}}\mathbf{Q}\vec{x} \\ &\text{subject to} && \mathbf{A}\vec{x} = \vec{1}_m. \end{aligned} \tag{7}$$

6.19. Development of a Normal Modes Analysis element for SAMSON platform

Participants: Yassine Naimi, Alexandre Hoffmann, Sergei Grudinin, Stephane Redon.

We are currently developing an element for the SAMSON platform for the calculation of normal modes based on the Normal Modes Analysis method. This element will be based on the program developed by Alexandre Hoffmann and Sergei Grudinin on Linux and Mac operating systems. First, we have ported the initial program from Linux and Mac operating systems to Windows and linked the program to the libraries needed for the calculations. These libraries consist in: an optimized version of BLAS (Basic Linear Algebra Subprograms) library called OpenBLAS for basic vector and matrix operations; LAPACK (Linear Algebra PACKage) library for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems; ARPACK library for solving large scale eigenvalue problems and ARMADILLO library which is a linear algebra library for the C++ language. We will also compare the performances of our program using these libraries to the Intel MKL (Math Kernel Library) libraries. The ultimate goal is to develop the interface for the SAMSON platform using the SAMSON SDK and Qt software.

6.20. Pairwise distance potential for protein folding

Participants: Maria Kadukova, Guillaume Pages, Alisa Patotskaya, Sergei Grudinin.

We have developed a new knowledge-based pairwise distance-dependent potential using convex optimization. This method uses histogram of distances repartition between each different pair of atom types as feature to feed an SVM-like algorithm. We then obtained a potential for each pair of atom types that can be used to score protein conformations. This method have been extensively used during the CASP12 blind assesement.

6.21. Knowledge-based scoring function for protein-ligand interactions

Participants: Maria Kadukova, Sergei Grudinin.

We have developed a knowledge-based pairwise distance-dependent scoring function based on the similar physical principles, as the protein folding potentials. It was trained on a set of protein-ligand complexes taken from the PDBBindCN database and validated on the CASF 2013 benchmark [50]. The corresponding paper submitted to Journal of Chemical Information and Modeling is currently under revision. We used this scoring function while participating in the 2015-2016 D3R Challenge.

6.22. Updates for the atomic typization software

Participants: Maria Kadukova, Sergei Grudinin.

We have additionally validated Knodle – our atomic typization software – on an extensive set of more than 300,000 small molecules based on the LigandExpo database. Knodle workflow involves machine-learning based "models" for different atoms, this year we retrained several of them on the updated version of PDBBindCN database. These results were published in Journal of Chemical Information and Modeling [45]. We also added functions that add missing hydrogen atoms to the molecules. Knodle was used to classify ligand atoms into different types in our protein-ligand interactions scoring function.

6.23. FFT-accelerated methods for fitting molecular structures into Cryo-EM maps

Participants: Alexandre Hoffmann, Sergei Grudinin.

We have developed a set of new methods for fitting molecular structures into Cryo-EM maps. The problem can be formally written as follows, We are given two proteins $\mathcal{P}_1$ and $\mathcal{P}_2$, and we also have $d_1 : \mathbb{R}^3 \to \mathbb{R}$, the electron density of $\mathcal{P}_1$ and $(Y_k)_{k=0 \cdots N_{atoms}-1}$, the starting positions of the atoms of $\mathcal{P}_2$. Assuming we can generate an artificial electron density $d_2 : \mathbb{R}^3 \to \mathbb{R}$ from $(Y_k)_{k=0 \cdots N_{atoms}-1}$, our problem is to find a transformation of the atoms $T : \mathbb{R}^3 \to \mathbb{R}^3$ that minimize the L^2 distance between d_1 and d_2.

In image processing this problem is usually solved using the optimal transport theory, but this method assumes that both of the densities have the same L^2 norm which is not necessarily the case for the fitting problem. To solve this problem, one instead starts by splitting T into a rigid transformation T_{rigid} (which is a combination of translation and rotation) and a flexible transformation $T_{flexible}$. Two classes of methods have been developed to find T_{rigid} :

- the first one uses optimization techniques such as gradient descent, and
- the second one uses Fast Fourier Transform (FFT) to compute the Cross Correlation Function (CCF) of d_1 and d_2.

The NANO-D team has already developed some algorithms based on the FFT to find T_{rigid} and we have been developing an efficient extension of these to find $T_{flexible}$.

6.24. Protein sequence and structure aligner for SAMSON

Participants: Guillaume Pages, Sergei Grudinin.

Aligning sequences and structures of proteins is important to understand both the homologies and differences between them. We developed a SAMSON element for this purpose, that can perform both sequence and structure alignment. The sequence alignment is done thanks to the software MUSCLE [36]. The structural alignment is done by finding the transformation that minimize the RMSD between corresponding backbones atoms in both structures. We used the algorithm presented by Kearsley [47].

6.25. Implementation of an Interactive Ramachandran Plot Element for SAMSON

Participants: Guillaume Pages, Sergei Grudinin.

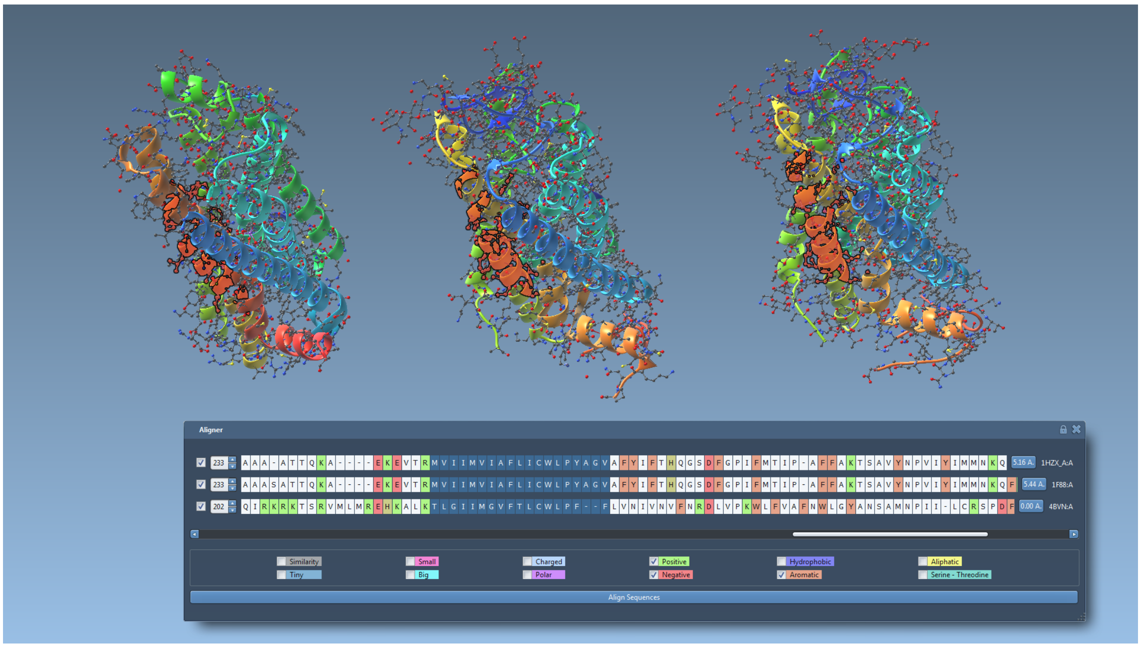


Figure 21. The protein aligner element

Each residue of a protein have two degrees of conformational freedom, described by the two dihedral angles of the backbone ϕ and ψ. Those two angles are crucial to visualize since they determine most of the protein backbone's overall conformation. A very useful way to represent them has been proposed by Ramachandran, Sasisekharan, and Ramakrishnan in 1963 [63].

We have developed a SAMSON element for displaying and editing the Ramachandran Plot of a protein. The favoured regions of the plot have been determined by analysing a database of high quality solved protein structure, provided on Richardson Lab's website (http://kinemage.biochem.duke.edu/databases/top8000.php).

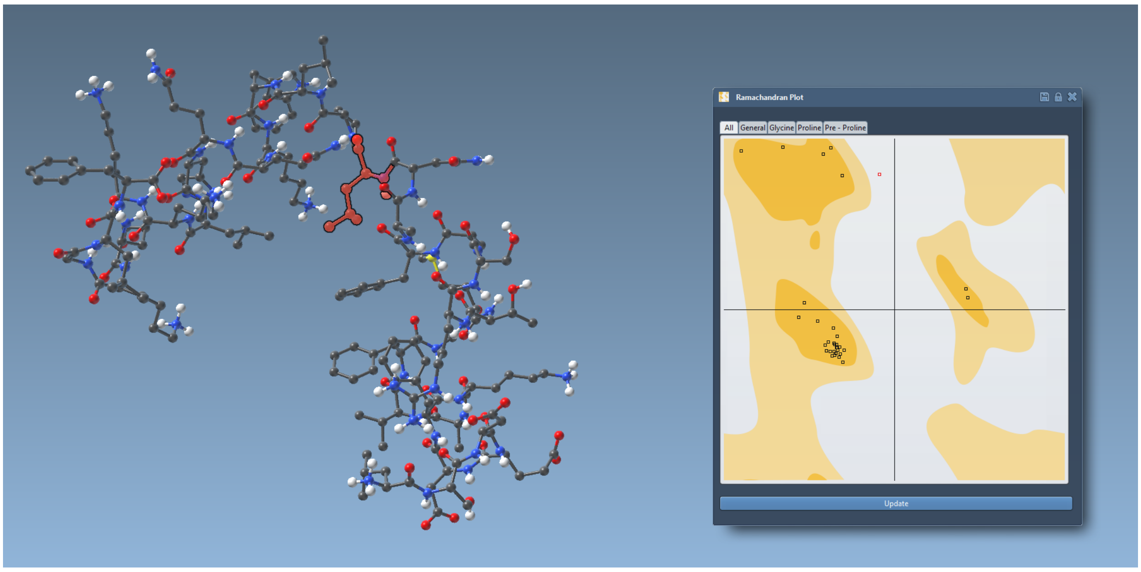


Figure 22. The Ramachandran plot element

POEMS Project-Team

7. New Results

7.1. New schemes for time-domain simulations

7.1.1. Solving the Homogeneous Isotropic Linear Elastodynamics Equations Using Potentials

Participant: Patrick Joly.

This work is done in collaboration with Sébastien Impériale (EPI M3DISIM) and Jorge Albella from the University of Santiago de Compostela. We consider the numerical solution of 2D elastodynamic equations using the decomposition of the displacement fields into potentials. This appears as a challenge for finite element methods. We address here the particular question of free boundary conditions. A stable (mixed) variational formulation of the evolution problem is proposed based on a clever choice of Lagrange multipliers. This is expected to be efficient when the velocity of shear waves is much smaller than the velocity of pressure waves, since one can adapt the discretization to each type of waves.

7.1.2. Discontinuous Galerkin method with high-order absorbing boundary conditions

Participant: Axel Modave.

This work is done in collaboration with Andreas Atle from TOTAL, Jesse Chan from Rice University and Tim Warburton from Virginia Tech.

Discontinuous Galerkin finite element schemes exhibit attractive features for large-scale time-domain wave-propagation simulations on modern parallel architectures (e.g. GPU clusters). For many applications, these schemes must be coupled with non-reflective boundary treatments to limit the size of the computational domain without losing accuracy or computational efficiency, which remains a challenging task.

We propose a combination of a nodal discontinuous Galerkin method with high-order absorbing boundary conditions (HABCs) for cuboidal computational domains. Compatibility conditions are derived for HABCs intersecting at the edges and the corners of a cuboidal domain. We propose a GPU implementation of the computational procedure, which results in a multidimensional solver with equations to be solved on 0D, 1D, 2D and 3D spatial regions. Numerical results demonstrate both the accuracy and the computational efficiency of our approach.

7.2. Integral equations

7.2.1. Mesh adaptation for the fast multipole method in acoustics

Participants: Faisal Amlani, Stéphanie Chaillat, Samuel Groth.

This work is done in collaboration with Adrien Loseille (EPI Gamma3). We introduce a metric-based anisotropic mesh adaptation strategy for the fast multipole accelerated boundary element method (FM-BEM) applied to exterior boundary value problems of the three-dimensional Helmholtz equation. The present methodology is independent of discretization technique and iteratively constructs meshes refined in size, shape and orientation according to an *optimal* metric reliant on a reconstructed Hessian of the boundary solution. The resulting adaptation is anisotropic in nature and numerical examples demonstrate optimal convergence rates for domains that include geometric singularities such as corners and ridges.

7.2.2. Coupling integral equations and high-frequency methods

Participants: Marc Bonnet, Marc Lenoir, Eric Lunéville, Laure Pesudo, Nicolas Salles.

This theme concerns wave propagation phenomena which involve two different space scales, namely, on the one hand, a medium scale associated with lengths of the same order of magnitude as the wavelength (medium-frequency regime) and on the other hand, a long scale related to lengths which are large compared to the wavelength (high-frequency regime). Integral equation methods are known to be well suited for the former, whereas high-frequency methods such as geometric optics are generally used for the latter. Because of the presence of both scales, both kinds of simulation methods are simultaneously needed but these techniques do not lend themselves easily to coupling.

A first situation, considered by Marc Lenoir, Eric Lunéville and Nicolas Salles, is the scattering of an acoustic wave by two sound-hard obstacles: a large obstacle subject to high-frequency regime relatively to the wavelength and a small one subject to medium-frequency regime. The technique proposed in this case consists in an iterative method which allows to decouple the two obstacles and to use Geometric Optics for the large obstacle and Boundary Element Method for the small obstacle. The method is implemented on the XLife++ library developed in the lab.

The second situation, undertaken in the context of the PhD thesis of Laure Pesudo, is the subject of a partnership with CEA LIST and a collaboration with Francis Collino. Modelling ultrasonic non destructive testing (NDT) experiments simultaneously involves the scattering of waves by defects of moderate size (for which discretization-based methods such as the BEM are appropriate) and propagation over large distances (requiring high-frequency approximations). A new hybrid strategy between the boundary element method (BEM) and ray tracing is proposed in order to allow the accurate and quick simulation of high frequency Non Destructive Testing (NDT) configurations involving diffraction phenomena. Results from its implementation to 2D acoustic NDT-like diffraction configurations have been obtained. The strategy proposed is however generic, and can be extended to three-dimensional configurations and elastodynamic wave propagation.

7.2.3. Dynamic soil-structure interaction

Participants: Marc Bonnet, Stéphanie Chaillat, Zouhair Adnani.

This work, undertaken in the context of the PhD thesis of Zouhair Adnani (CIFRE partnership with EDF), concerns the simulation of dynamic soil-structure interaction (SSI) in connection with seismic assessment of civil engineering structures. Because of the complementary specificities of the finite element method (FEM) and the boundary element method (BEM), it is natural to use the BEM to model the unbounded soil domain, while the FEM is applied for the bounded region comprising the structure undergoing assessment, and possibly its close-range soil environment.

The originality of this work is to formulate, implement, and evaluate on realistic test examples, a computational strategy that combines the fast multipole accelerated boundary element method (visco-elastodynamic COFFEE solver), and the EDF in-house FEM code Code_Aster. In a preliminary phase, the evaluation of transient elastodynamic responses via the Fourier synthesis of frequency domain solutions computed using COFFEE (see Section 5.1) has been studied on several test problems, achieving substantial improvements of computational efficiency for this component of SSI analysis.

The coupling between the two methods is then done in a black-box fashion with the substructuring method by computing the soil impedance (i.e. elastodynamic Poincaré-Steklov) operator relating forces to displacements on the FEM-BEM coupling interface. One of the main challenges is that this operator cannot be assembled due to the iterative nature of the FM-BEM and the potentially large number of degrees of freedom supported by the interface. To reduce the computational costs, we instead compute its projection on a reduced basis of interface modes, which requires to perform as many FM-BEM calculations as interface modes selected. This approach has so far been compared to reference solutions and validated for superficial and buried foundations on homogeneous or heterogeneous soil.

7.2.4. Volume Integral Formulations

Participant: Marc Bonnet.

Volume integral equations (VIEs), also known as Lippmann-Schwinger integral equations, arise naturally when considering the scattering of waves by penetrable, and possibly heterogeneous, inhomogeneities embedded in a homogeneous background medium (for which a fundamental solution is explicitly known). Their derivation and use in e.g. acoustics, elastodynamics or electromagnetism goes back several decades. Since their geometrical support is confined to the spatial region where material properties differ from the background, VIEs are in particular useful for the derivation and justification of homogenized or asymptotic models (the latter providing our main motivation for this study, in connection with [section gradient topologique]). By directly linking remote measurements to unknown inhomogeneities, VIEs also provide a convenient forward modeling approach for medium imaging inverse problems. However, whereas the theory of boundary integral equations is extensively documented, the mathematical properties of VIEs have undergone a comparatively modest coverage, much of it pertaining to electromagnetic scattering problems.

In this work, we investigate the solvability of VIE formulations arising in elastodynamic scattering by penetrable obstacles. The elasticity tensor and mass density are allowed to be smoothly heterogeneous inside the obstacle and may be discontinuous across the background-obstacle interface, the background elastic material being homogeneous. Both materials may be anisotropic, within certain limitations for the background medium.

Towards this goal, we have introduced a modified version of the singular volume integral equation (SVIE) governing the corresponding elastostatic (i.e. zero frequency) problem, and shown it to be of second kind involving a contraction operator, i.e. solvable by Neumann series, for any background material and inhomogeneity material and geometry. Then, the solvability of VIEs for frequency-domain elastodynamic scattering problems follows by a compact perturbation argument, assuming uniqueness to be established. In particular, in an earlier work, we have established a uniqueness result for the anisotropic background case (where, to avoid difficulties associated with existing radiation conditions for anisotropic elastic media, we have proposed an alternative definition of the radiating character of solutions, which is equivalent to the classical Sommerfeld-Kupradze conditions for the isotropic background case). This investigation extends work by Potthast (1999) on 2D electromagnetic problems (transverse-electric polarization conditions) involving orthotropic inhomogeneities in a isotropic background, and contains recent results on the solvability of Eshelby's equivalent inclusion problem as special cases. The proposed modified SVIE is also useful for fixed-point iterative solution methods, as Neumannn series then converge (i) unconditionally for static problems and (ii) on some inhomogeneity configurations for which divergence occurs with the usual SVIE for wave scattering problems.

7.3. Domain decomposition methods

7.3.1. Transparent boundary conditions with overlap in unbounded anisotropic media

Participants: Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss, Yohanes Tjandrawidjaja.

This work is done in the framework of the PhD of Yohanes Tjandrawidjaja, funded by CEA-LIST, in collaboration with Vahan Baronian form CEA. This follows the PhD of Antoine Tonnoir (now Assistant Professor at Insa of Rouen) who developed a new approach, the Half-Space Matching Method, to solve scattering problems in 2D unbounded anisotropic media. The objective is to extend the method to a 3D plate of finite width.

In 2D, our approach consists in coupling several plane-waves representations of the solution in half-spaces surrounding the defect with a FE computation of the solution around the defect. The difficulty is to ensure that all these representations match, in particular in the infinite intersections of the half-spaces. It leads to a Fredholm formulation which couples, via integral operators, the solution in a bounded domain including the defect and some traces of the solution on the edge of the half-planes.

The extension to 3D elastic plates requires some generalizations of the formulation which are not obvious. In particular, we have to use Neumann traces of the solution, which raises difficult theoretical questions.

As a first step, we have considered a scattering problem outside a convex polygonal scatterer for a general class of boundary conditions, using the Half-Space Matching Method. Using the Mellin Transform, we are able to show that this system is coercive + compact in presence of dissipation.

Let us mention that the Half-Space Matching Method has been extended successfully by Julian Ott (Karlsruhe Institut für Technologie) to the scattering by junctions of open waveguides in 2D.

7.3.2. Domain Decomposition Methods for the neutron diffusion equation

Participants: Patrick Ciarlet, Léandre Giret.

This work is done in collaboration with Erell Jamelot (CEA-DEN, Saclay) and Félix Kpadonou (LMV, UVSQ). Studying numerically the steady state of a nuclear core reactor is expensive, in terms of memory storage and computational time. In its simplest form, one must solve a neutron diffusion equation with low-regularity solutions, discretized by mixed finite element techniques, within a loop. Iterating in this loop allows to compute the smallest eigenvalue of the system, which determines the critical, or non-critical, state of the core. This problem fits within the framework of high performance computing so, in order both to optimize the memory storage and to reduce the computational time, one can use a domain decomposition method, which is then implemented on a parallel computer: this is the strategy used for the APOLLO3 neutronics code. The development of non-conforming DD methods for the neutron diffusion equation with low-regularity solutions has recently been finalized, cf. [PC,EJ,FK'1x]. The theory for the eigenvalue problem is also understood. The current research now focuses on the numerical analysis of the full suite of algorithms to prove convergence for the complete multigroup SPN model (which involves coupled diffusion equations).

7.4. Wave propagation in complex media

7.4.1. Perfectly Matched Layers in plasmas and metamaterials

Participants: Eliane Bécache, Maryna Kachanovska.

In this work we consider the problem of the modelling of 2D anisotropic dispersive wave propagation in unbounded domains with the help of perfectly matched layers (PML). We study the Maxwell equations in passive media with the frequency-dependent diagonal tensor of dielectric permittivity and magnetic permeability. An application of the traditional PMLs to this kind of problems often results in instabilities, due to the presence of so-called backward propagating waves. In previous works, this instability was overcome with the help of the frequency-dependent correction of the PML, for isotropic dispersive models.

We show that this idea can be extended to a more general class of models (uniaxial cold plasma, some anisotropic metamaterials). Crucially, we base our considerations on the Laplace-domain techniques. This allows to avoid the analysis of the group and phase velocity (used before) but study (rather formally) coercivity properties of the sesquilinear form corresponding to the PML model in the Laplace domain. The advantage of this method is that it permits to treat problems with dissipation, and provides an intuition on how to obtain explicit energy estimates for the resulting PML models in the time domain. However, such analysis does not allow to obtain easily the necessary stability condition of the PML. We demonstrate that the necessary stability conditions of the PML can be rewritten for a class of models in a form that is easy to verify, and demonstrate that these conditions are sufficient for the stability of the new PMLs with the help of the Laplace-domain techniques. Thanks to the Laplace domain analysis, we are able to rewrite a PML system in the time domain in a form, for which the derivation of energy estimates is simplified (compared to other formulations).

7.4.2. Transparent Boundary Conditions for the Wave Propagation in Fractal Trees

Participants: Patrick Joly, Maryna Kachanovska.

This work, done in collaboration with Adrien Semin (Postdoctoral student at the Technische Universität of Berlin), is dedicated to an efficient resolution of the wave equation in self-similar trees (e.g. wave propagation in a human lung). In this case it is possible to avoid computing the solution at deeper levels of the tree by using the transparent boundary conditions. The corresponding DtN operator is defined by a functional equation in the frequency domain. In this work we propose and compare two approaches to the discretization of this operator in the time domain. The first one is based on the multistep convolution quadrature, while the second one stems from the rational approximations.

7.4.3. High order transmission conditions between homogeneous and homogenized periodic half-spaces

Participants: Sonia Fliss, Valentin Vinoles.

This work is a part of the PhD of Valentin Vinoles, and is done in collaboration with Xavier Claeys from Paris 6 University and EPI ALPINE. It is motivated by the fact that classical homogenization theory poorly takes into account interfaces, which is particularly unfortunate when considering negative materials, because important phenomena arise precisely at their surface (plasmonic waves for instance). To overcome this limitation, we want to construct high order transmission conditions. For now, we have treated the case of a plane interface between a homogeneous and a periodic half spaces. Using matched asymptotic techniques, we have derived high order transmission conditions. We have then introduced an approximate model associated to this asymptotic expansions which consists in replacing the periodic media by an effective one but the transmission conditions are not classical. The obtained conditions involve Laplace- Beltrami operators at the interface and requires to solve cell problems in periodicity cell (as in classical homogenisation) and in infinite strips (to take into account the phenomena near the interface). We establish well posedness for the approximate and error estimate which justify that this new model is more accurate near the interface and in the bulk. From a numerical point of view, the only difficulty comes from the problems set in infinite strips (one half is homogeneous and the other is periodic). This is overcome using DtN operators corresponding to the homogeneous and the periodic media.The numerical results confirm the theoretical ones.

7.4.4. Finite Element Heterogeneous Multiscale Method for Maxwell's Equations

Participants: Patrick Ciarlet, Sonia Fliss.

This work is done in collaboration with Christian Stohrer (Karlsruhe Institute of Technology, Allemagne). In recent years, the Finite Element Heterogeneous Multiscale Method (FE-HMM) has been used to approximate the effective behavior of solutions to PDEs in highly oscillatory media. We started on the extension of the FE-HMM to the Helmholtz equation in such media, and recently we solved the time-harmonic Maxwell equations case. Using a combination of results regarding the FE-HMM and the notion of T-coercivity applied to Maxwell's equations, we derive an a priori error bound and the error. Moreover, numerical experiments corroborate the analytical findings, cf. [PC,SF,CS'1x].

7.5. Spectral theory and modal approaches for waveguides

7.5.1. Plasmonic waveguides

Participants: Anne-Sophie Bonnet-Ben Dhia, Patrick Ciarlet.

This work is done in collaboration with Camille Carvalho (UC Merced, California, USA) and Lucas Chesnel (EPI DEFI). A plasmonic waveguide is a cylindrical structure consisting of metal and dielectric parts. In a certain frequency range, the metal can be seen as a lossless material with a negative dielectric permittivity. The study of the modes of a plasmonic waveguide is then presented as a model eigenvalue problem with a sign-change of coefficients in the main part of the operator. Depending on the values of the contrast of permittivities at the metal/dielectric interface, different situations may occur. We focus on the situation where the interface between metal and dielectric presents corners. For a particular contrast range, the problem is neither self-adjoint nor with compact resolvent, this is the "critical" case. Whereas in the "nice" case, the problem is self-adjoint with compact resolvent and admits two sequences of eigenvalues tending to $-\infty$ and $+\infty$. In the "critical" case, Kondratiev's theory of singularities allows to build extensions of the operator, with compact resolvent. We show that the eigenvalues for one of these extensions can be computed by combining finite elements and Perfectly Matched Layers at the corners. The paradox is that a specific treatment has to be done to capture the corners singularities, even to compute regular eigenmodes. In the "nice" case, we propose and analyze numerical techniques based on the notion of T-coercive meshes that allow to solve the model problem.

7.5.2. Modal analysis of electromagnetic dispersive media

Participants: Christophe Hazard, Sandrine Paolantoni.

We investigate the spectral effects of an interface between a usual dielectric and a negative-index material (NIM), that is, a dispersive material whose electric permittivity and magnetic permeability become negative in some frequency range. We consider here an elementary situation, namely, 1) the simplest existing model of NIM : the Drude model (for which negativity occurs at low frequencies); 2) a two-dimensional scalar model derived from the complete Maxwell's equations; 3) the case of a simple bounded cavity: a camembert-like domain partially

lled with a portion of non dissipative Drude material. Because of the frequency dispersion (the permittivity and permeability depend on the frequency), the spectral analysis of such a cavity is unusual since it yields a nonlinear eigenvalue problem. Thanks to the use of an additional unknown, we show how to linearize the problem and we present a complete description of the spectrum.

7.5.3. Formulation of invisibility in waveguides as an eigenvalue problem

Participants: Antoine Bera, Anne-Sophie Bonnet-Ben Dhia.

This work is done in collaboration with Lucas Chesnel from EPI DEFI, Vincent Pagneux from Laboratoire d'Acoustique de l'Université du Maine and Sergei Nazarov from Russian Academy of Sciences. A scatterer placed in an infinite waveguide may be *invisible* at particular discrete frequencies. We consider two different definitions of invisibility: no reflection (but possible conversion or phase shift in transmission) or perfect invisibility (the scattered field is exponentially decaying at infinity). Our objective is to show that the invisibility frequencies can be characterized as eigenvalues of some spectral problems. Two different approaches will be used for the two different definitions of invisibility, leading to non-selfadjoint eigenvalue problems. Concerning the non-reflection case, our approach based on an original use of PMLs allows to extend to higher dimension and to complex eigenvalues the results obtained by Hernandez-Coronado, Krejcirik and Siegl on a 1D model problem.

7.5.4. Transparent boundary conditions for general waveguide problems

Participants: Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss.

In this work, done in collaboration with Antoine Tonnoir from INSA of Rouen, we propose a construction of transparent boundary conditions which can be used for quite general waveguide problems. Classical Dirichlet-to-Neumann maps used for homogeneous acoustic waveguides can be constructed using separation of variables and the orthogonality of the modes on one transverse section. These properties are also important for the mathematical and numerical analysis of problems involving DtN maps. However this framework does not extend directly to strati

ed, anisotropic or periodic waveguides and for Maxwell's or elastic equations. The difficulties are that (1) the separation of variables is not always possible and (2) the modes of the waveguides are not necessarily orthogonal on the transverse section. We propose an alternative to the DtN maps which uses two artificial boundaries and is constructed using a more general orthogonality property.

7.6. Inverse problems

7.6.1. Linear Sampling Method with realistic data in waveguides

Participants: Laurent Bourgeois, Arnaud Recoquillay.

Our activities in the field of inverse scattering in waveguides with the help of sampling methods has now a quite long history. We now intend to apply these methods in the case of realistic data, that is surface data in the time domain. This is the subject of the PhD of Arnaud Recoquillay. It is motivated by Non Destructive Testing activities for tubular structures and is the object of a partnership with CEA List (Vahan Baronian).

Our strategy consists in transforming the time domain problem into a multi-frequency problem by the Fourier transform. This allows us to take full advantage of the established efficiency of modal frequency-domain sampling methods. We have already proved the feasibility of our approach in the 2D acoustic and 2D elastic case. In particular, we have shown how to optimize the number of sources/receivers and the distance between them in order to obtain the best possible identification result. Experiments are currently carried in CEA.

7.6.2. The “exterior approach" to solve inverse obstacle problems

Participants: Laurent Bourgeois, Arnaud Recoquillay.

We consider some inverse obstacle problems in acoustics by using a single incident wave, either in the frequency or in the time domain. When so few data are available, a Linear Sampling type method cannot be applied. In order to solve those kinds of problem, we propose an “exterior approach", coupling a mixed formulation of quasi-reversibility and a simple level set method. In such iterative approach, for a given defect D, we update the solution u with the help of a mixed formulation of quasi-reversibility while for a given solution u, we update the defect D with the help of a level set method based on a Poisson problem. The case of data in the frequency domain has been studied for the waveguide geometry. We currently investigate the case of data in a finite time domain.

7.6.3. Topological derivatives of leading- and second-order homogenized coefficients.

Participants: Marc Bonnet, Rémi Cornaggia.

This work is done in collaboration with Bojan Guzina from University of Minnesota. We derive the topological derivatives of the homogenized coefficients associated to a periodic material, with respect of the small size of a penetrable inhomogeneity introduced in the unit cell that defines such material. In the context of antiplane elasticity, this work extends existing results to (i) time-harmonic wave equation and (ii) second-order homogenized coefficients, whose contribution reflects the dispersive behavior of the material.

7.6.4. A continuation method for building large invisible obstacles in waveguides

Participants: Antoine Bera, Anne-Sophie Bonnet-Ben Dhia.

In collaboration with Lucas Chesnel (EPI DEFI) and Sergei Nazarov (Saint-Petersburg University), we consider time harmonic acoustic problems in waveguides. We are interested in finding localized perturbations of a straight waveguide which are not detectable in the far field, as they produce neither reflection nor conversion of propagative modes. In other words, such *invisible* perturbation produces a scattered field which is exponentially decaying at infinity in the two infinite outlets of the waveguide.

In our previous contributions, we found a way to build smooth and small perturbations of the boundary which were almost invisible, in the sense that they were producing no reflexions but maybe a phase shift in transmission.

The method is constructive and has been validated numerically. But the drawback is that it is limited to small perturbations. In the present work, we show that the previous idea can be combined with a continuation method, in order to get larger invisible perturbations.

7.7. Aeroacoustics

7.7.1. Time-harmonic acoustic scattering in a vortical flow

Participants: Antoine Bensalah, Patrick Joly, Jean-François Mercier.

This activity is done in the framework of the PhD of Antoine Bensalah, in partnership with Airbus Group. We study the time-harmonic acoustic radiation in a fluid in a general flow which is not curl free, but has restricted vortical areas. The objective is to take into account the complicated coupling between acoustics and hydrodynamics. The Galbrun approach developed previously in 2D is too expensive in terms of degrees of freedom for 3D simulations. As an alternative, we propose to consider instead the Goldstein equations, which are vectorial only in the vortical areas and remain scalar elsewhere.

To begin with, we aim at determining the acoustic field radiated in 2D by a time-harmonic source in a fluid in flow. Goldstein's equations are proved to be well-posed outside a spectrum of frequencies corresponding to resonant streamlines. This band spectrum is explicitly determined for two simple geometries (an annular domain and a rectangular one with periodic conditions). Then the full model is shown to be well-posed under a coercivity condition, implying a subsonic flow with a small enough vorticity.

7.7.2. Propagation of solitons through Helmholtz resonators

Participant: Jean-François Mercier.

With Bruno Lombard (Laboratoire de Mécanique et Acoustique of Marseille), we study the propagation of nonlinear solitary acoustic waves in a 1D waveguide connected to a lattice of Helmholtz resonators. We start from an homogenized model of the literature, consisting of two coupled equations evolution: a nonlinear PDE describing acoustic waves (similar to the Burgers equation), and a linear ODE describing oscillations in the Helmholtz resonators. We have already developed a numerical modeling of this model and we have compared simulations with experimental data.

The drawback of the homogenized model is that all the resonators must be the same. In particular the reflection of an incident wave by a defect cannot be considered. To remedy this limitation, we have proposed an extension of the model, predicting two-way propagation across variable resonators. Thanks to a new discrete description of the resonators, the improved model takes into account two important features: resonators of different strengths and back-scattering effects. Comparisons with experimental data show that a closer agreement is obtained.

RAPSODI Team

7. New Results

7.1. large-time behavior of some numerical schemes

In [19], C. Chainais-Hillairet, A. Jüngel and S. Schuchnigg prove the time decay of fully discrete finite-volume approximations of porous-medium and fast-diffusion equations with Neumann or periodic boundary conditions in the entropy sense. The algebraic or exponential decay rates are computed explicitly. In particular, the numerical scheme dissipates all zeroth-order entropies which are dissipated by the continuous equation. The proofs are based on novel continuous and discrete generalized Beckner inequalities.

In [13], M. Bessemoulin-Chatard and C. Chainais-Hillairet study the large-time behavior of a numerical scheme discretizing drift-diffusion systems for semiconductors. The numerical method is based on a generalization of the classical Scharfetter-Gummel scheme which allows to consider both linear or nonlinear pressure laws.They study the convergence of approximate solutions towards an approximation of the thermal equilibrium state as time tends to infinity, and obtain a decay rate by controlling the discrete relative entropy with the entropy production. This result is proved under assumptions of existence and uniform-in-time L^∞ estimates for numerical solutions, which are then discussed.

The question of uniform-in-time L^∞ estimates for the scheme proposed in [13] has then be tackled by M. Bessemoulin-Chatard, C. Chainais-Hillairet and A. Jüngel. The result is obtained *via* a Moser's iteration technique adapted to the discrete setting. Related to this question, the existence of a positive lower bound for the numerical solution of a convection-diffusion equation has been studied by C. Chainais-Hillairet, B. Merlet and A. Vasseur. They apply a method due to De Giorgi in order to establish a positive lower bound for the numerical solution of a stationary convection-diffusion equation. These results are submitted for publication in the FVCA8 conference (to be held in June 2017).

In [11] B. Merlet *et al.* consider a second-order two-step time discretization of the Cahn-Hilliard equation with an analytic nonlinearity. They study the long time behavior of the discrete solution and show that if the time-step is chosen small enough, the sequence generated by the scheme converges to a steady state as time tends to infinity. Convergence rates are also provided. This parallels the behavior of the solutions of the non-discretized solutions and shows the reliability of the scheme for long time simulations. The method of proof is based on the Lojasiewicz-Simon inequality and on the study of the pseudo-energy associated with the discretization which is shown to be non-increasing.

7.2. Theoretical and numerical analysis of corrosion models

The Diffusion Poisson Coupled Model [1] is a model of iron based alloy in a nuclear waste repository. It describes the growth of an oxide layer in this framework. The system is made of a Poisson equation on the electrostatic potential and convection-diffusion equations on the densities of charge carriers (electrons, ferric cations and oxygen vacancies). The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations. Numerical experiments done for the simulation of this model with moving boundaries show the convergence in time towards a pseudo-steady-state. C. Chainais-Hillairet and T. O. Gallouët prove in [18] the existence of pseudo-stationary solutions for some simplified versions of the DPCM model. They also propose a new scheme in order to compute directly this pseudo-steady-state. Numerical experiments show the efficiency of this method.

The modeling of concrete carbonation also leads to a system of partial differential equations posed on a moving domain. C. Chainais-Hillairet, B. Merlet and A. Zurek propose and analyze a finite volume scheme for the concrete carbonation model. They prove the convergence of the sequence of approximate solutions towards a weak solution. Numerical experiments show the order 2 in space of the scheme and illustrate the $\sqrt{t}$ law of propagation of the size of the carbonated zone. This result is submitted for publication.

7.3. Modeling and numerics for porous media flows

In [16], C. Cancès and C. Guichard propose a nonlinear Control Volume Finite Elements method with upwinding in order to solve possibly nonlinear and degenerate parabolic equations. This method was designed in order to preserve at the discrete level the positivity and the nonlinear stability of the solutions. In [25], A. Ait Hammou Oulhaj, C. Cancès, and C. Chainais-Hillairet extend the approach of [16] to the more complex case of Richards equation modeling saturated/unsaturated flows in anisotropic porous media. The additional complexity comes from the fact that convective terms and elliptic degeneracy are considered in [25]. The scheme preserves at the discrete level the nonnegativity and the nonlinear stability of the solutions. Its convergence is rigorously proved, and numerical results are provided in order to illustrate the behavior of the scheme.

In [49], C. Cancès, T. O. Gallouët, and L. Monsaingeon show that the equations governing two-phase flows in porous media have a formal gradient flow structure. The goal of the longer contribution [29] is then twofold. First, it extends the variational interpretation of [49] to the case where an arbitrary number of phases are in competition to flow within a porous medium. Second, we provide rigorous foundations to our claim. More precisely, the convergence of a minimizing movement scheme *à la* Jordan, Kinderlehrer, and Otto [66] is shown in [29], providing by the way a new existence result for multiphase flows in porous media. The result relies on advances tools related to optimal transportation [75], [74].

7.4. Complex fluid flows: modeling, analysis and numerics

The analysis of the Kazhikhov-Smagulov model was given by Bresch at al. [48] (see also reference therein). These authors prove the global existence of weak solution without assuming small data and without any assumption on the diffusivity coefficient. Following the physical experiment given by Joseph [67], we introduce a Korteweg stress tensor in the previous model. The theory of Korteweg considers the possibility that motions can be driven by additional stresses associated with gradients of density. In process of slow diffusion on miscible incompressible fluids, for example water and glycerin, dynamical effects which mimic surface tension can arise in thin mixing layers where the gradients of density are large. In the context of the PhD thesis of Meriem Ezzoug (July 2016, University of Monastir, Tunisia), C. Calgaro and co-authors study a multiphase incompressible fluid model, called the Kazhikhov-Smagulov-Korteweg model. They prove in [14] that this model is globally well posed in a 3D bounded domain.

In [21], P.-E. Jabin and T. Rey investigate the behavior of granular gases in the limit of small Knudsen number, that is very frequent collisions. They deal with the physically relevant strongly inelastic case, in one dimension of space and velocity. The study of such limit, also known as hydrodynamic limit is to give a reduced description of the kinetic equation, using a fluid approximation. They are able to prove the convergence of the particle distribution function toward a monokinetic distribution, whose moments verify the pressureless Euler system. The proof relies on dispersive relations at the kinetic level, which leads to the so-called Oleinik property at the limit, and in particular stability of the solution to the fluid problem.

In [34], I. Lacroix-Violet and A. Vasseur present the construction of global weak solutions to the quantum Navier-Stokes equation, for any initial value with bounded energy and entropy. The construction is uniform with respect to the Planck constant. This allows to perform the semi-classical limit to the associated compressible Navier-Stokes equation. One of the difficulty of the problem is to deal with the degenerate viscosity, together with the lack of integrability on the velocity. The method is based on the construction of weak solutions that are renormalized in the velocity variable. The existence, and stability of these solutions do not need the Mellet-Vasseur inequality [71].

In [31], G. Dimarco, R. Loubère, J. Narski and T. Rey deal with the extension of the Fast Kinetic Scheme (FKS) [55], [56] originally constructed for solving the BGK equation, to the more challenging case of the Boltzmann equation. The scheme combines a robust and fast method for treating the transport part based on an innovative Lagrangian technique supplemented with fast spectral schemes to treat the collisional operator by means of an operator splitting approach. This approach along with several implementation features related to the parallelization of the algorithm permits to construct an efficient simulation tool which is numerically tested against exact and reference solutions on classical problems arising in rarefied gas dynamic. They present results up to the 3D×3D case for unsteady flows for the Variable Hard Sphere model which may serve as benchmark. For this reason, they also provide for each problem details on the computational cost and memory consumption as well as comparisons with the BGK model or the limit model of compressible Euler equations.

7.5. Improving the numerical efficiency of numerical methods

In this section, we gather contributions in which a methodology was introduced in order to reduce the computational cost at fixed accuracy or to improve the accuracy for a fixed computational cost.

In [20], E. Creusé and his collaborators generalized some of their previous results on residual a posteriori error estimators for low electromagnetism [10] , [52] to the case where some voltage or current excitation is specified in the model (see e.g. such models in [63], [42]). It consequently led to consider different formulations and to overcome some specific difficulties in order to derive the reliability of the involved estimators.

It is now well accepted that well-balanced schemes are of great interest in order to compute accurate solutions to systems of PDEs (see for instance [60]). In [36], L. Pareschi and T. Rey propose a systematic way to tune classical numerical schemes in order to make them well-balanced and asymptotic preserving. Inspired by micro-macro decomposition methods for kinetic equations, they present a class of schemes which are capable to preserve the steady state solution and achieve high order accuracy for a class of time dependent partial differential equations including nonlinear diffusion equations and kinetic equations. Extension to systems of conservation laws with source terms are also discussed, as well as Total Variation Diminishing preserving properties.

The contribution [26] by K. Brenner and C. Cancès is devoted to the improvement of the behavior of Newton's method when solving degenerate parabolic equations. Such equations are very common for instance in the context of complex porous media flows. In [26], the presentation focuses on Richards equation modeling saturated/unsaturated flows in porous media. The basic idea is the following: Newton's method is not invariant by nonlinear change of variables. The choice of the primary variable then impacts the effective resolution of the nonlinear system provided by the scheme. The idea developed in [26] is then to construct an abstract primary variable to facilitate Newton's method's convergence. This leads to an impressive reduction of the computational cost, a better accuracy in the results and an strong robustness of the method w.r.t. the nonlinearities appearing in the continuous model.

7.6. Variational modeling and analysis

Bose-Einstein condensates are a unique way to observe quantum effects at a (relatively) large scale. The fundamental states of such condensates are obtained as minimizers of a Gross-Pitaievskii functional. In [33], M. Goldman and B. Merlet consider the case of a two component Bose-Einstein condensate in the strong segregation regime (the energy favors spatial segregation of the two different Boson species). They identify two different regimes in the strong segregation and small healing length limit. In one of these regimes, the relevant limit is an interesting weighted isoperimetric problem which explains some of the numerical simulations of [70].

In [32], B. Merlet *et al.* consider the branched transportation problem in 2D associated with a cost per unit length of the form $1 + \alpha m$ where m denotes the amount of transported mass and $\alpha > 0$ is a fixed parameter (the limit case $\alpha = 0$ corresponds to the classical Steiner problem). Motivated by the numerical approximation of this problem, they introduce a family of functionals ($\{F_\varepsilon\}_{\varepsilon>0}$) which approximate the above branched transport energy. They justify rigorously the approximation by establishing the equicoercivity and the Γ-convergence of F_ε as $\varepsilon \downarrow 0$. These functionals are modeled on the Ambrosio-Tortorelli functional and are easy to optimize in practice (the algorithm amounts to perform repetitively the alternate optimization of two quadratic functionals). Numerical evidences of the efficiency of the method are presented.

7.7. Miscellaneous

This section gathers results from members of the team that are not directly related to the core of the scientific program of the team.

In [12], I. Violet-Lacroix and co-authors consider the derivation of continuous and fully discrete artificial boundary conditions for the linearized Korteweg-de-Vries equation. They are provided for two different numerical schemes. The boundary conditions being nonlocal with respect to time variable, they propose fast evaluations of discrete convolutions. Various numerical tests are presented to show the effectiveness of the constructed artificial boundary conditions.

A semi-discrete in time Crank-Nicolson scheme to discretize a weakly damped forced nonlinear fractional Schrödinger equation in the whole space ($\mathbb{R}$ is considered by C. Calgaro and co-authors in [28]. They prove that such semi-discrete equation provides a discrete infinite dimensional dynamical in $H^\alpha(\mathbb{R})$ that possesses a global attractor. They show also that if the external force is in a suitable weighted Lebesgue space then this global attractor has a finite fractal dimension.

In [35], F. Nabet considers a finite-volume approximation, based on a two point flux approximation, for the Cahn-Hilliard equation with dynamic boundary conditions. An error estimate for the fully-discrete scheme on a possibly smooth non-polygonal domain is proved and numerical simulations which validate the theoretical result are given.

APICS Project-Team

5. New Results

5.1. Inverse problems for Poisson-Laplace equations

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Konstantinos Mavreas, Christos Papageorgakis, Dmitry Ponomarev.

This section is concerned with inverse problems for 3-D Poisson-Laplace equations, among which source recovery issues. Though the geometrical settings differ in Sections 5.1.1 and 5.1.5 , the characterization of silent sources (those giving rise to a vanishing field) is one common problem to both cases. The latter has been resolved in the magnetization setup for thin slabs [36]. The case of volumetric distribution is currently being investigated, starting with magnetization distributions on closed surfaces to which the general volumetric case can be reduced by balayage.

5.1.1. Inverse magnetization issues in the thin-plate framework

This work is carried out in the framework of the Inria Associate Team IMPINGE, comprising Eduardo Andrade Lima and Benjamin Weiss from the Earth Sciences department at MIT (Boston, USA) and Douglas Hardin, Michael Northington, Edward Saff and Cristobal Villalobos from the Mathematics department at Vanderbilt University (Nashville, USA).

The overall goal of IMPINGE is to determine magnetic properties of rock samples (*e.g.* meteorites or stalactites) from weak field measurements close to the sample that can nowadays be obtained using SQUIDs (superconducting quantum interference devices). During previous years, we always considered the case when the rock is cut into slabs so thin that the magnetization distribution could be considered to lie in a plane. This year, we started considering the situation where the thickness r of the sample cannot be ignored. The thin-slab case thus appears as a limiting case when r goes to 0.

Figure 3 presents a schematic view of the experimental setup: the sample lies on a horizontal plane at height 0 and its support is included in a parallelepiped. The vertical component B_3 of the field produced by the sample is measured on points of a horizontal square at height z.

We focused on net moment recovery, the net moment of a magnetization being given by its mean value on the sample. The net moment is a valuable piece of information to Physicists and has the advantage of being well-defined: whereas two different magnetizations can generate the same field, the net moment depends only on the field and not on the magnetization itself. Hence the goal may be described as building a numerical magnetometer, capable of analyzing data close to the sample. This is in contrast to classical magnetometers which regard the latter as a single dipole, an approximation which is only valid away from the sample and is not suitable to handle weak fields which get quickly blurred by ambient magnetic sources. This research effort was paid in two different, complementary directions.

The first approach consists in computing asymptotic expansions of the integrals $\iint B_3(x_1,x_2,z)\,\mathrm{d}x_1\mathrm{d}x_2$, $\iint x_1\,B_3(x_1,x_2,z)\,\mathrm{d}x_1\mathrm{d}x_2$ and $\iint x_2\,B_3(x_1,x_2,z)\,\mathrm{d}x_1\mathrm{d}x_2$, on several domains (namely, the 2-D balls of radius R for the 1, 2 and ∞ norm, that are squares, disks, diamonds), in terms of the moments of first and higher order of the magnetization m. Last year, we obtained formulas valid only under the thin-slab hypothesis. This year, we extended the results to the case of a volumetric magnetization. We posted a preprint [22] with these results on HAL, and our partners at MIT are currently conducting practical experiments with the SQUID to illustrate the method, before submitting it to some journal. In parallel, Fourier based techniques designed by reformulating the problem with the help of the Kelvin transform also furnish an asymptotic expansion of the net moment involving, at the first order, the above-mentioned integrals computed on disks of large radius. The computations are quite involved but allow to obtain higher-order terms. This constitutes Part III of D. Ponomarev's PhD work [11], defended this year.

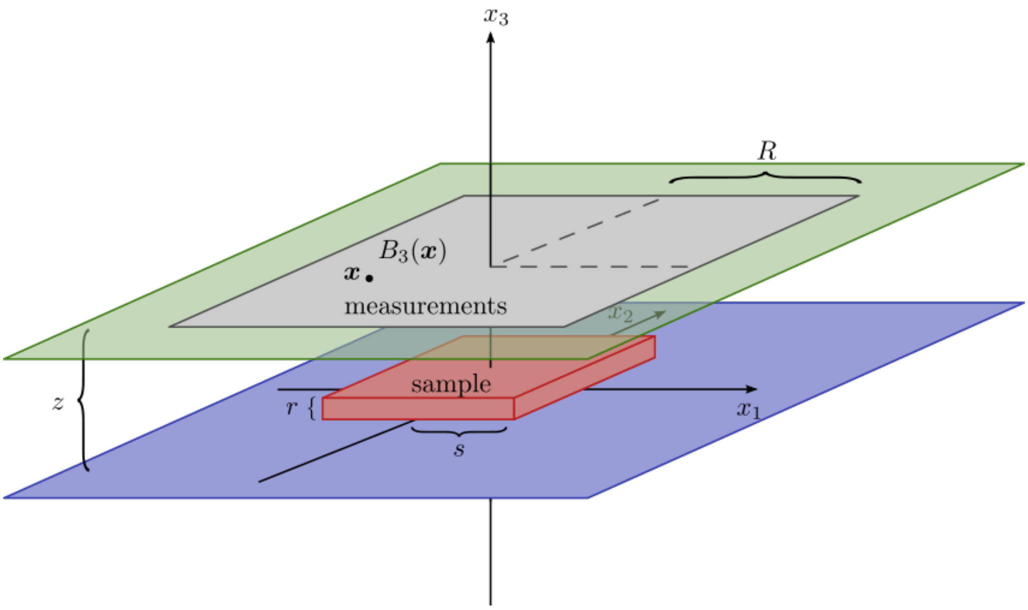


Figure 3. Schematic view of the experimental setup

The second approach attempts to generalize the previous expansions. The initial question is: given measurements of B_3, find a function $\phi(x_1, x_2)$ such that $\iint \phi(x_1, x_2) B_3(x_1, x_2)\, \mathrm{d}x_1 \mathrm{d}x_2$ is best possible an estimate of the net moment components $\langle m_i \rangle$ $(i = 1, 2, 3)$, in some appropriate sense. This problem has no solution really because, for any $\epsilon > 0$, there exists a function ϕ_ϵ allowing to estimate the moment with an error bounded by ϵ. We proved that, when ϵ tends to zero, the norm of the function ϕ_ϵ tends to infinity, which hinders an accurate numerical computation of the integral since B_3 is only known on a discrete grid of points. We therefore expressed the problem as a bounded extremal problem (see Section 3.3.1): to find the best ϕ_ϵ (with the smallest possible error value ϵ) under the constraint that $\|\nabla \phi_\epsilon\|_2 \leq M$. Here, M is a user-defined parameter. We improved on the iterative algorithm devised last year and completed the theoretical justification of its convergence. Basic properties of the operators involved, which are necessary to carry out the procedure, have been derived in [21], along with perspectives on minimum L^2 regularization for the computation of local moments (which are usually not determined by the field, unlike the net moment).

We also performed preliminary numerical experiments which are very encouraging, but still need to be pushed further in connection with the delicate issue of how dense should the grid of data points be in order to reach a prescribed level of precision. An article on this topic is in preparation.

In this connection, the PhD thesis of D. Ponomarev's [11], Part II, contains a study of the 2D spectral problem for the truncated Poisson operator in planar geometry. This is a simplified (*i.e.* 2-D) setup for the relation between the magnetization and the magnetic potential, of which the magnetic field is the gradient. It is relevant because, by the familiar Courant min-max principle, the eigenvectors of the magnetization-to-field operator produce in principle an efficient basis to expand a given magnetization in short series. Describing these eigenvectors is a long-standing problem. Asymptotic formulas as the measurement height gets small with respect to the size of the sample have been obtained, both for dominant eigenvalues and eigenvectors, through connections with other spectral problems. In fact, asymptotic reductions for large and small values of the main parameters (distance h from the measurement plane to the sample support and sample support size), yield approximate solutions by means of simpler integral equations and ODEs.

5.1.2. Inverse magnetization issues from sparse spherical data

The team Apics is a partner of the ANR project MagLune on Lunar magnetism, headed by the Geophysics and Planetology Department of Cerege, CNRS, Aix-en-Provence (see Section 7.2.2). Recent studies let geoscientists to think that the Moon used to have a magnetic dynamo for a while, yet the exact process that triggered and fed this dynamo is still not understood, much less why it stopped. The overall goal of the project is to devise models to explain how this dynamo phenomenon was possible on the Moon.

The geophysicists from Cerege went this year to NASA to perform measurements on a few hundreds of samples brought back from the Moon by Apollo missions. The samples are kept inside bags with a protective atmosphere, and geophysicists are not allowed to open the bags, nor to take out samples from NASA facilities. Moreover, the process must be carried out efficiently as a fee is due to NASA by the time when handling these moon samples. Therefore, measurements were performed with some specific magnetometer designed by our colleagues from Cerege. This device measures the components of the magnetic field produced by the sample, at some discrete set of points located on circles belonging to three cylinders (see Figure 4). The objective of Apics is to enhance the numerical efficiency of post-processing data obtained with this magnetometer.

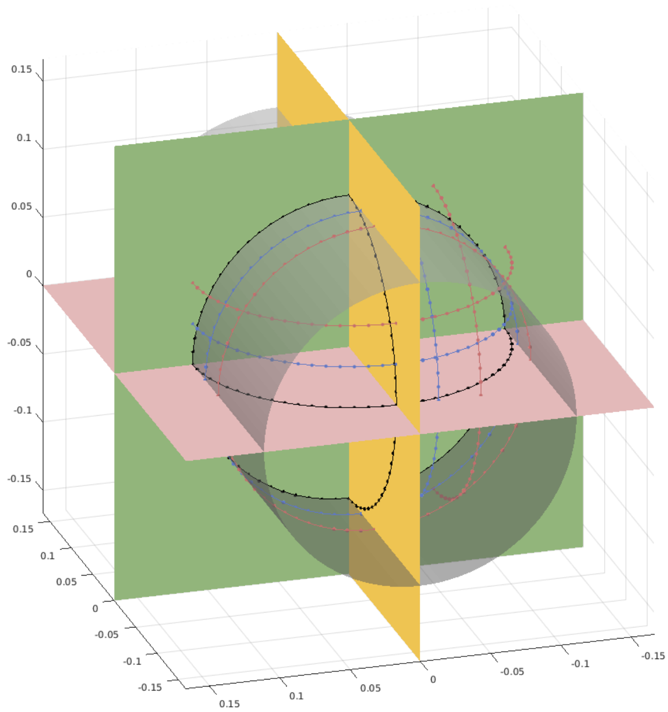


Figure 4. Typical measurements obtained with the instrument of Cerege. Measurements of the field are performed on nine circles, given as sections of three cylinders. On each circle, only one component of the field is measured: the component B_h along the axis of the corresponding cylinder (blue points), the component B_n radial with respect to the circle (black points), or the component B_τ tangential to the circle (red points).

This year, we continued the approach initiated in 2015 during K. Mavreas' internship: under the hypothesis that the field can be well explained by a single magnetic dipole, and using ideas similar to those underlying the FindSources3D tool (see Sections 3.4.2 and 5.1.5), we try to recover the position and moment of the dipole. The rational approximation technique that we are using gives, for each circle of measurements, a partial information about the position of the dipole. These partial informations obtained on all nine circles must then be combined in order to recover the exact position. Theoretically speaking, the nine partial informations are redundant and the position could be obtained by several equivalent techniques. But in practice, due to the fact that the field is not truly generated by a single dipole, and also because of noise in the measurements and numerical errors in the rational approximation step, all methods do not show the same reliability when combining the partial results. We studied several approaches, testing them on synthetic examples, with more or less noise, in order to propose a good heuristic for the reconstruction of the position. This is still on-going work.

5.1.3. Surface distributed magnetizations and vector fields decomposition

This is a joint work with Pei Dang and Tao Qian from the University of Macao.

Silent magnetizations in the thin plate case were characterized in [36] using a decomposition of $\mathbb{R}^3$-valued vector fields defined on $\mathbb{R}^2 \sim \mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$. More precisely, in rather general smoothness classes (involving all distributions with compact support), such a vector field is the sum of the traces on $\mathbb{R}^2$ of a harmonic gradient in the upper half space, a harmonic gradient in the lower half space, and of a tangential divergence-free vector field. This year the corresponding decomposition has been obtained in L^p-classes on closed surfaces, where $1 < p < \infty$ if the surface is smooth but p has to be restricted around the value 2 if the surface is only Lipschitz smooth. The proof uses elliptic regularity theory, some Hodge theory and Clifford analysis.

In the case where the curvature is constant (*i.e.* for spheres and planes), one recovers using the previous result that silent distribution have no inner harmonic gradient component, whereas in the case of more general surfaces one finds they have to satisfy a spectral equation for the double layer potential. This also furnishes a characterization of volumetric silent distributions by saying that their balayage to the boundary of the volume (which is a closed surface) is silent. An article is being written on this topic.

5.1.4. Decomposition of the geomagnetic field

This is a joint work with Christian Gerhards from the University of Vienna.

The techniques based on solving bounded extremal problems, set forth in Section 5.1.1 to estimate the net moment of a planar magnetization, may be used to approach the problem of decomposing the magnetic field of the Earth into its crustal and core components, when adapted to a spherical geometry.

Indeed, in geomagnetism it is of interest to separate the Earth's core magnetic field from the crustal magnetic field. However, satellite measurements can only sense the superposition of the two contributions. In practice, the measured magnetic field is expanded in terms of spherical harmonics and a separation into crust and core contribution is done empirically by a sharp cutoff in the spectral domain. Under the assumption that the crustal magnetic field is supported on a strict subset of the Earth's surface, which is nearly verified as some regions on the globe are only very weakly magnetic, one can state an extremal problem to find a linear form yielding an arbitrary coefficient of the expansion in spherical harmonics on the crustal field, while being nearly zero on the core contribution. An article is being prepared to report on this research.

5.1.5. Inverse problems in medical imaging

This work is conducted in collaboration with Jean-Paul Marmorat and Nicolas Schnitzler, together with Maureen Clerc and Théo Papadopoulo from the Athena EPI.

In 3-D, functional or clinically active regions in the cortex are often modeled by pointwise sources that have to be localized from measurements, taken by electrodes on the scalp, of an electrical potential satisfying a Laplace equation (EEG, electroencephalography). In the works [6], [41] on the behavior of poles in best rational approximants of fixed degree to functions with branch points, it was shown how to proceed via best rational approximation on a sequence of 2-D disks cut along the inner sphere, for the case where there are finitely many sources (see Section 4.3).

In this connection, a dedicated software FindSources3D (see Section 3.4.2) is being developed, in collaboration with the team Athena and the CMA. In addition to the modular and ergonomic platform version of FindSources3D, a new (Matlab) version of the software that automatically performs the estimation of the quantity of sources is being built. It uses an alignment criterion in addition to other clustering tests for the selection. It appears that, in the rational approximation step, *multiple* poles possess a nice behavior with respect to branched singularities. This is due to the very physical assumptions on the model (for EEG data, one should consider *triple* poles). Though numerically observed in [7], there is no mathematical justification so far why multiple poles generate such strong accumulation of the poles of the approximants. This intriguing property, however, is definitely helping source recovery. It is used in order to automatically estimate the "most plausible" number of sources (numerically: up to 3, at the moment). Last but not least, this new version may take as inputs actual EEG measurements, like time signals, and performs a suitable singular value decomposition in order to separate independent sources.

In connection with these and other brain exploration modalities like electrical impedance tomography (EIT), we are now studying conductivity estimation problems. This is the topic of the PhD research work of C. Papageorgakis (co-advised with the Athena project-team and BESA GmbH). In layered models, it concerns the estimation of the conductivity of the skull (intermediate layer). Indeed, the skull was assumed until now to have a given isotropic constant conductivity, whose value can differ from one individual to another. A preliminary issue in this direction is: can we uniquely recover and estimate a single-valued skull conductivity from one EEG recording? This has been established in the spherical setting when the sources are known, see [14]. Situations where sources are only partially known and the geometry is more realistic than a sphere are currently under study. When the sources are unknown, we should look for more data (additional clinical and/or functional EEG, EIT, ...) that could be incorporated in order to recover both the sources locations and the skull conductivity. Furthermore, while the skull essentially consists of a hard bone part, which may be assumed to have constant electrical conductivity, it also contains spongy bone compartments. These two distinct components of the skull possess quite different conductivities. The influence of the second on the overall model is currently being studied.

5.2. Matching problems and their applications

Participants: Laurent Baratchart, Martine Olivi, David Martinez Martinez, Fabien Seyfert.

This is collaborative work with Stéphane Bila (XLIM, Limoges, France), Yohann Sence (XLIM, Limoges, France), Thierry Monediere (XLIM, Limoges, France), Francois Torrès (XLIM, Limoges, France) in the context of the ANR Cocoram (see Section 7.2.1).

Filter synthesis is usually performed under the hypothesis that both ports of the filter are loaded on a constant resistive load (usually 50 Ohm). In complex systems, filters are however cascaded with other devices, and end up being loaded, at least at one port, on a non purely resistive frequency varying load. This is for example the case when synthesizing a multiplexer: each filter is here loaded at one of its ports on a common junction. Thus, the load varies with frequency by construction, and is not purely resistive either. Likewise, in an emitter-receiver, the antenna is followed by a filter. Whereas the antenna can usually be regarded as a resistive load at some frequencies, this is far from being true on the whole pass-band. A mismatch between the antenna and the filter, however, causes irremediable power losses, both in emission and transmission. Our goal is therefore to develop a method for filter synthesis that allows us to match varying loads on specific frequency bands, while enforcing some rejection properties away from the pass-band.

Figure 5 shows a filter with scattering matrix S, plugged at its right port on a frequency varying load with reflection parameter $L_{1,1}$. If the filter is lossless, simple algebraic manipulations show that on the frequency axis the reflex-ion parameter satisfies:

$$|G_{1,1}| = \left| \frac{S_{2,2} - \overline{L_{1,1}}}{1 - S_{2,2} L_{1,1}} \right| = \delta(G_{1,1}, S_{2,2}).$$

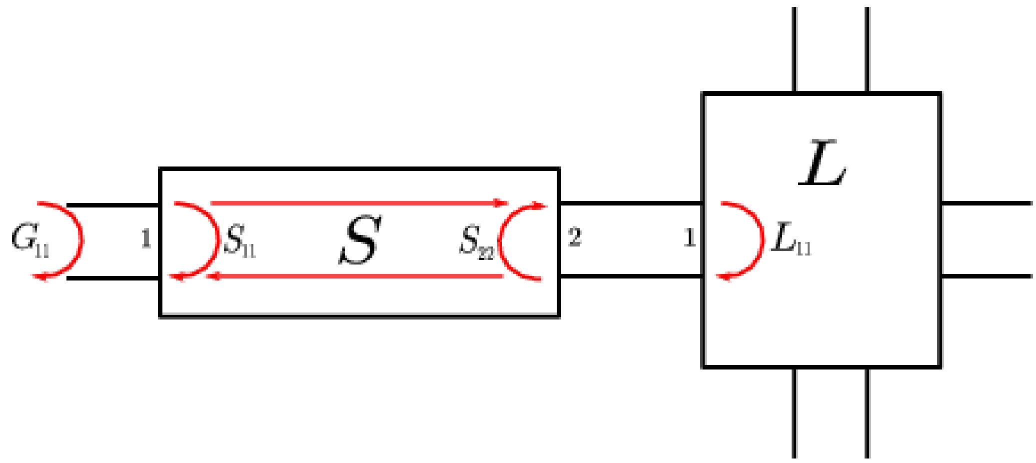


Figure 5. Filter plugged on a system with reflexion coefficient L_{11}

The matching problem of minimizing $|G_{1,1}|$ amounts therefore to minimize the pseudo-hyperbolic distance δ between the filter's reflex-ion parameter $S_{2,2}$ and the load's reflex-ion $L_{1,1}$, on a given frequency band. On the contrary enforcing a rejection level on a stop band, amounts to maintaining the value of $\delta(L_{1,1}, S_{2,2})$ above a certain threshold on this frequency band. For a broad class of filters, namely those that can be modeled by a circuit of n coupled resonators, the scattering matrix S is a rational function of McMillan degree n in the frequency variable. The matching problem thus appears to be a rational approximation problem in the hyperbolic metric.

5.2.1. Approach based on interpolation

When the degree n of the rational function $S_{2,2}$ is fixed, the hyperbolic minimization problem is non-convex which leads us to seek methods to derive good initial guesses for classical descent algorithms. To this effect, if $S_{2,2} = p/q$ where p, q are polynomials, we considered the following interpolation problem $\mathcal{P}$: given n frequency points $w_1 \cdots w_n$ and a transmission polynomial r, to find a monic polynomial p of degree n such that:

$$j = 1..n, \qquad \frac{p}{q}(w_j) = \overline{L_{1,1}(w_j)}$$

where q is the unique monic Hurwitz polynomial of degree n satisfying the Feldtkeller equation

$$qq^* = pp^* + rr^*,$$

which accounts for the losslessness of the filter. The frequencies (w_k) are perfect matching points where $\delta(S_{2,2}(w_k), L_{1,1}(w_k)) = 0$ holds, while the real zeros (x_k) of r are perfect rejection points (i.e. $\delta(S_{2,2}(x_k), L_{1,1}(x_k)) = 1$). The interpolation problem is therefore a point-wise version of our original matching-rejection problem. The monic restriction on p and q ensures the realizability of the filter in terms of coupled resonating circuits. If a perfect phase shifter is added in front of the filter, realized for example with a transmission line on a narrow frequency band, these monic restrictions can be dropped and an extra interpolation point w_{n+1} is added, thereby yielding another interpolation problem $\widehat{\mathcal{P}}$. Our main result, states that $\mathcal{P}$ as well as $\widehat{\mathcal{P}}$ admit a unique solution. Moreover the evaluation map defined by $\psi(p) = (p/q(x_1), \cdots, p/q(x_n))$ is a homeomorphism from monic polynomials of degree n onto $\mathbb{D}^n$ ($\mathbb{D}$ the complex open disk), and ψ^{-1} is a diffeomorphism on an open, connected, dense set of $\mathbb{D}^n$. This last property has shown to be crucial for the design of an effective computational procedure based on continuation techniques. Current implementations of the latter tackle instances of $\mathcal{P}$ or $\widehat{\mathcal{P}}$ for $n = 10$ in less than 0.1 sec, and allow for a recursive use of this interpolation framework in multiplexer synthesis problems. We presented these techniques at the MTNS conference 2016 held in Mineapolis [17]. The detailed mathematical proofs can be found in [23] which is under review at SIMA, the SIAM journal on Mathematical Analysis.

5.2.2. Uniform matching and global optimality considerations

The previous interpolation procedure provides us with a matching/rejecting filtering characteristics at a discrete set of frequencies. This may serve as a starting point for heavier optimization procedures, where the matching and rejection specifications are expressed uniformly over the bandwidth. Although the practical results thus obtained have shown to be quite convincing, we have no proof of their global optimality. This led us to seek alternative approaches able to assess, at least in simple cases, global optimality of the derived response. By optimality we mean, as in classical filtering, the ability to derive the uniformly best matching response in a given pass-band, while ensuring some rejection constraints on a stop-band. Following the approach of Fano and Youla, we considered the problem of designing a 2×2 loss-less frequency response, under the condition that a specified load can be "unchained" from one of its port. This classically amounts to set interpolation conditions on the response at the transmission zeros of the Darlington extension of the load. When the load admits a rational representation of degree 1, and if the transmission zeros of the overall system are fixed, then we were able to show that the uniform matching problem over an interval, together with rejection constraints at other frequency locations, reduces to a convex minimization problem with convex constraints over the set of non-negative polynomials of given degree. In this case, which is already of some practical interest for antenna matching (antennas usually exhibit a single resonance in their matching band which is decently approximated at order 1), it is therefore possible to perform filter synthesis with a guarantee on the global optimality of the obtained characteristics. The practical approach, relying on convex duality and linear programming is presented in [26], together with an implementation using a SIW (substrate integrated filter).

5.3. Sensitivities of Electrical Parameters with respect to physical parameters

Participants: Matthias Caenepeel, Martine Olivi, Fabien Seyfert.

This work was conducted in collaboration with Yves Rolain (VUB, Brussels, Belgium). The goal is to automatize and improve our computer-aided tuning (CAT) method for coupled-resonator microwave synthesis, which is based on rational approximation and circuit extraction as explained before. The novelty here lies with estimating the Jacobian of the function that relates the physical filter design parameters to the extracted coupling parameters. Lately commercial full-wave electromagnetic (EM) simulators provide the adjoint sensitivities of the S-parameters with respect to the geometrical parameters. This information allows us for an efficient estimation of the Jacobian since it no longer requires finite difference based evaluation. Our tuning method first extracts the physically implemented coupling matrix, and then estimates the corresponding Jacobian. Next it compares the extracted coupling matrix to the target coupling matrix (golden goal). Using the difference between the coupling matrices and the pseudo-inverse of the estimated Jacobian, a correction that brings the design parameters closer to the golden goal is obtained. This process is repeated iteratively until the correction becomes sufficiently small with respect to a user-specified goal. In the case of coupling structures with multiple solutions, the Jacobian is calculated for each admissible solution. This paper presents a criterion to identify the physical solution among the different possibilities. The CAT method has been applied to the design of a cascaded triplet (CT) filter implemented in a microstrip technology. This filter is a well-known examples of a non-canonical coupling structure. See [24] for details.

5.4. Stability of amplifiers

Participants: Laurent Baratchart, Sylvain Chevillard, Martine Olivi, Fabien Seyfert, Sebastien Fueyo.

This work is performed under contract with CNES-Toulouse and the University of Bilbao as well as in collaboration with Adam Cooman (VUB, Brussels, Belgium). The goal is to help design amplifiers, in particular to detect instability at an early stage of the design. Activity in this area is gaining importance with the coming of a doctoral and a postdoctoral student along with planned software developments.

Performing a stability analysis during the design of any electronic circuit is critical to guarantee its correct operation. A closed-loop stability analysis can be performed by analyzing the impedance presented by the circuit at a well-chosen node without internal access to the simulator. If any of the poles of this impedance lie in the complex right half-plane, the circuit is unstable. The classic way to detect unstable poles is to fit a rational model on the impedance. This rational approximation has to deal with model order selection, which is difficult in circuits with transmission lines. In the practical approach we develop in collaboration with Adam Cooman, a projection-based method is proposed which splits the impedance into a stable and an unstable part by projecting on an orthogonal basis of stable and unstable functions. Working with a projection instead of a rational approximation greatly simplifies the stability analysis. When the projection is mapped from the complex plane to the unit disc, it boils down to calculating a Fourier series. If a significant part of the impedance is projected on the unstable part, a low-order rational approximation is fitted on this unstable part to find the location of the unstable poles. See [25] for details. Adapting such tools to check the stability of a trajectory, linearizing around the latter, is tantamount to develop a similar theory for time-varying periodic systems. This is the subject of S. Fueyo's PhD work.

5.5. Tools for numerically guaranteed computations

Participant: Sylvain Chevillard.

The overall and long-term goal is to enhance the quality of numerical computations. The software tool Sollya (see Section 3.4.5), developed together with C. Lauter (Université Pierre et Marie Curie) intends to provide an interactive environment for performing numerically rigorous computations. During year 2016, we released version 5.0 (in June) and version 6.0 (in October) of Sollya. Among other things, these releases have heavily improved the internal handling of polynomial expressions and the speed of the faithful evaluation of functions. They also make the library API more complete and fix most of the reported bugs. Another important novelty of 2016 is that Sollya is now officially included in the Debian Linux distribution.

5.6. Asymptotics of weighted Bergman polynomials

Participant: Laurent Baratchart.

We extended this year exterior asymptotics for orthonormal polynomials with respect to a weight on a planar region Ω (so-called weighted Bergman polynomials) to the case where Ω is simply connected, asymptotically conformal and chord arc, with exterior conformal map f from the complement of the disk to the complement of Ω such that f''/f' lies in a Hardy class H^q with $q<1$. This class of domain is more general than, say the $C^{1\alpha}$ class. Meanwhile the weight should have integrable non-tangential maximal function and non-tangential limit with positive geometric mean. As $n\to\infty$, the formula reads

$$P_n(z)=\left(\frac{n+1}{\pi}\right)^{1/2} S_{w\circ f}(\Phi(z))\,\Phi^n(z)\Phi'(z)\{1+o(1)\},$$

locally uniformly outside the convex hull of Ω, where $\Phi=f^{-1}$ and $S_{w\circ f}$ is the Szegő function of the boundary weight . The proof uses quasi-conformal mappings and some Hardy space theory, along with classical Fourier analysis of Taylor sections.

The result goes much beyond those previously known, which either assume analyticity of Ω or else constant or analytic weight. An article is being written on this topic.

BIPOP Project-Team

6. New Results

6.1. The contact complementarity problem, and Painlevé paradoxes

Participants: Bernard Brogliato, Florence Bertails-Descoubes, Alejandro Blumentals.

The contact linear complementarity problem is an set of equalities and complementarity conditions whose unknowns are the acceleration and the contact forces. It has been studied in a frictionless context with possibly singular mass matrix and redundant constraints, using results on well-posedness of variational inequalities obtained earlier by the authors. This is also the topic of the first part of the Ph.D. thesis of Alejandro Blumentals where the frictional case is treated as a perturbation of the frictionless case [22]. With R. Kikuuwe from Kyushu University, we have also proposed a new formulation of the Baumgarte's stabilisation method, for unilateral constraints and Coulomb's friction , which sheds new light on Painlevé paradoxes [27]. It relies on a particular limiting process of normal cones.

6.2. Discrete-time sliding mode control

Participants: Vincent Acary, Bernard Brogliato, Olivier Huber.

This topic concerns the study of time-discretized sliding-mode controllers. Inspired by the discretization of nonsmooth mechanical systems, we propose implicit discretizations of discontinuous, set-valued controllers [3]. This is shown to result in preservation of essential properties like simplicity of the parameters tuning, suppression of numerical chattering, reachability of the sliding surface after a finite number of steps, and disturbance attenuation by a factor h or h^2 [25]. This work was part of the ANR project CHASLIM. Within the framework of CHASLIM we have performed many experimental validations on the electropneumatic setup of IRCCyN (Nantes), which nicely confirm our theoretical and numerical predictions: the implicit implementation of sliding mode control, drastically improves the input and output chattering behaviours, both for the classical order-one ECB-SMC and the twisting algorithms [26], [25], [39]. In particular the high frequency bang-bang controllers which are observed with explicit discretizations, are completely suppressed. The implicit discretization has been applied to the classical equivalent-based-control SMC, and also to the twisting sliding-mode controller. Incidentally an error in a previous article is corrected in [19]. The previous results deal with disturbances which are matched and uniformly upperbounded. In [48], [49] they are extended to the case of parametric uncertainties, which are more difficult to handle because they may yield unmatched equivalent disturbances, and these disturbances are not uniformly upperbounded by a constant. Finally the results in [20] deal with the numerical analysis (and not the discrete-time control, which is a different problem) of Lagrangian systems with set-valued controllers. An implicit Euler method is used, and the convergence is shown.

6.3. Lur'e set-valued dynamical systems

Participants: Bernard Brogliato, Christophe Prieur, Alexandre Vieira.

Lur'e systems are quite popular in Automatic Control since the fifties. Set-valued Lur'e systems possess a static feedback nonlinearity that is a multivalued function. We study in [31] state observers for particular Lur'e systems which are Moreau's sweeping processes modelling Lagrange dynamics with frictionless unilateral constraints. The observers are themselves set-valued (first order sweeping process with measures), a complete analysis (existence of solutions, stability of the error system) is led. In [51], we extend previous results in the team and also more recently by Camlibel and Schumacher, to solve the problem of output regulation for evolution variational inequalities (in a convex analysis setting). In the PhD thesis of A. Vieira, we attack the problem of optimal control of linear complementarity systems. In the first part of this thesis, the case when the LCS is equivalent to an ODE with Lipschitz continuous right-hand side, is treated. Starting from first-order necessary conditions stated in a broad context by Clarke, we show that the Pontryagin's conditions are a mixed LCS, that yield so-called MPEC problems.

6.4. Numerical analysis of multibody mechanical systems with constraints

This scientific theme concerns the numerical analysis of mechanical systems with bilateral and unilateral constraints, with or without friction [2]. They form a particular class of dynamical systems whose simulation requires the development of specific simulators.

6.4.1. Numerical time–integration methods for event-detecting schemes.

Participants: Vincent Acary, Bernard Brogliato, Mounia Haddouni.

The CIFRE thesis of M. Haddouni concerns the numerical simulation of mechanical systems subject to holonomic bilateral constraints, unilateral constraints and impacts. This work is performed in collaboration with ANSYS and the main goal is to improve the numerical time–integration in the framework of event-detecting schemes. Between nonsmooth events, time integration amounts to numerically solving a differential algebraic equations (DAE) of index 3. We have compared dedicated solvers (Explicit RK schemes, Half-explicit schemes, generalizes α-schemes) that solve reduced index formulations of these systems. Since the drift of the constraints is crucial for the robustness of the simulation through the evaluation of the index sets of active contacts, we have proposed some recommendations on the use of the solvers of dedicated to index-2 DAE. A manuscript has been submitted to Multibody System Dynamics.

6.4.2. Multibody systems with clearances (dynamic backlash)

Participants: Vincent Acary, Bernard Brogliato, Narendra Akadkhar.

The PhD thesis of N. Akadkhar under contract with Schneider Electric concerns the numerical simulation of mechanical systems with unilateral constraints and friction, where the presence of clearances in imperfect joints plays a crucial role. A first work deals with four-bar planar mechanisms with clearances at the joints, which induce unilateral constraints and impacts, rendering the dynamics nonsmooth. The objective is to determine sets of parameters (clearance value, restitution coefficients, friction coefficients) such that the system's trajectories stay in a neighborhood of the ideal mechanism (*i.e.* without clearance) trajectories. The analysis is based on numerical simulations obtained with the projected Moreau-Jean time-stepping scheme. These results have been reported in [21]. It is planned to extend these simulations to frictional cases and to mechanisms of circuit breakers.

6.5. Nonlinear waves in granular chains

Participants: Guillaume James, Bernard Brogliato.

Granular chains made of aligned beads interacting by contact (e.g. Newton's cradle) are widely studied in the context of impact dynamics and acoustic metamaterials. While much effort has been devoted to the theoretical and experimental analysis of solitary waves in granular chains, there is now an increasing interest in the study of breathers (spatially localized oscillations) in granular systems. Due to their oscillatory nature and associated resonance phenomena, static or traveling breathers exhibit much more complex dynamical properties compared to solitary waves. Such properties have strong potential applications for the design of acoustic metamaterials allowing to efficiently damp or deviate shocks and vibrations. In the work [29], the existence of static breathers is analyzed in granular metamaterials consisting of hollow beads with internal masses. Using multiple scale analysis and exploiting the unilateral character of Hertzian interactions, we show that long-lived breather solutions exist but time-periodic breathers do not (breather solutions actually disperse on long time scales). In [28], we consider the effect of adding precompression to the above system and establish that the envelope of small ampliude oscillations is governed by a nonlinear Schrödinger equation. This allows us to show that, depending on the applied precompression, normal modes can become modulationally unstable and evolve towards traveling breathers. Moreover, in a collaboration with Y. Starosvetsky and D. Meimukhin (Technion), we numerically study the persistence of traveling breathers in granular chains with local potentials under the effect of contact damping. Using a viscoelastic damping model (Hertz-Kuwabara-Kono model), we show that breathers can be generated by simple impacts in granular chains made from various materials (breathers propagate over a significant number of sites before being damped). The design of an experimental setup to test these theoretical predictions is underway. Another work in progress concerns more specifically the modeling and numerical analysis of dissipative impacts (James, Brogliato). The methodology is based on the introduction of appropriate variables and simplifications for different models of contact damping. A postdoctoral fellow will work on this topic in the team, starting January 2017.

6.6. Travelling waves in a spring-block chain sliding down a slope

Participants: Guillaume James, Jose Eduardo Morales Morales, Arnaud Tonnelier.

In this work we study the dynamics of an infinite chain of identical blocks sliding on a slope under the effet of gravity. Each block is coupled to its nearest neighbour through linear springs and is subjected to a nonlinear friction force. For a piecewise-linear spinodal friction law, a closed-form expression of front waves is derived. Pulse waves are obtained as the matching of two travelling fronts with identical wave speeds. Explicit formulas are obtained for the wavespeed and the wave form in the anti-continuum limit. The link with propagating phenomena in the Burridge-Knopoff model is briefly discussed. These results have been reported in [44].

6.7. Solitary waves in the excitable Burridge-Knopoff model

Participants: Guillaume James, Jose Eduardo Morales Morales, Arnaud Tonnelier.

The Burridge-Knopoff model is a lattice differential equation describing a chain of blocks connected by springs and pulled over a surface. This model was originally introduced to investigate nonlinear effects arising in the dynamics of earthquake faults. One of the main ingredients of the model is a nonlinear velocity-dependent friction force between the blocks and the fixed surface. For some classes of non-monotonic friction forces, the system displays a large response to perturbations above a threshold, which is characteristic of excitable dynamics. Using extensive numerical simulations, we show that this response corresponds to the propagation of a solitary wave for a broad range of friction laws (smooth or nonsmooth) and parameter values. These solitary waves develop shock-like profiles at large coupling (a phenomenon connected with the existence of weak solutions in a formal continuum limit) and propagation failure occurs at low coupling. We introduce a simplified piecewise linear friction law (reminiscent of the McKean nonlinearity for excitable cells) which allows us to obtain analytical expression of solitary waves and study some of their qualitative properties, such as wavespeed and propagation failure. We propose a possible physical realization of this system as a chain of impulsively forced mechanical oscillators. In certain parameter regimes, non-monotonic friction forces can also give rise to bistability between the ground state and limit-cycle oscillations and allow for the propagation of fronts connecting these two stable states. These results have been reported in [45]. In addition, an existence theorem for solitary waves in the Burridge-Knopoff model is proved in the weak coupling limit and for a piecewise-linear friction force.

6.8. Propagation in space-discrete excitable systems

Participant: Arnaud Tonnelier.

We introduce a simplified model of excitable systems where the response of an isolated cell to an incoming signal is described by a fixed pulse-shape function. When the total activity of the cell reaches a given threshold a signal is sent to its N nearest neighbors. We show that a chain of such excitable cells is able to propagate a set of simple traveling waves where the time interval between the firing of two successive cells remains constant. A comprehensive study is done for a transmission line with $N = 2$ and $N = 3$. It is shown that, depending on initial copnditions, the network may propagate signals with different velocities. Some necessary conditions for multistationarity are derived for an arbitrary N.

6.9. Direct and inverse modeling of thin elastic rods and shells

6.9.1. Experimental validation of the inverse statics of a thin elastic rod

Participants: Florence Bertails-Descoubes, Victor Romero.

In collaboration with Arnaud Lazarus (UPMC, Laboratoire Jean le Rond d'Alembert), we have built an experimental set-up to fabricate thin elastic rods and measure their deformation, with the aim to validate our full process for inverse static design. This work is still ongoing.

6.9.2. Strain-based modeling of inextensible and developable shells

Participants: Florence Bertails-Descoubes, Romain Casati, Alejandro Blumentals.

We have worked out the analagous of a super-helix element for modeling an inextensible and developable shell patch, using only two material curvatures. As for the super-helix model, the terms of the dynamics can be integrated formally, leading to a rich and efficient dynamical model [36]. How to connect different patches together is a topic for future work.

6.9.3. Inverse statics of plates and shells with frictional contact

Participants: Florence Bertails-Descoubes, Romain Casati, Gilles Daviet.

We study the problem of cloth inverse design, relying on a nodal shell model for modeling garments. We have shown how to formulate draping as a local constrained minimization problem, and we have generalized the adjoint method to handle constrained cases, e.g., frictional contact between the garment and the body [43].

6.10. Continnum modeling of granular materials

6.10.1. Continuum modeling of granular materials

Participants: Florence Bertails-Descoubes, Gilles Daviet.

We have proposed a new numerical framework for the continuous simulation of dilatable materials with pressure-dependent (Coulomb) yield stress, such as sand or cement. Relying upon convex optimization tools, we have shown that the continuous equations of motion coupled to the macroscopic nonsmooth Drucker-Prager rheology can be interpreted as the exact analogous of the solid frictional contact problem at the heart of Discrete Element Methods (DEM), extended to the tensorial space. Combined with a carefully chosen finite-element discretization, this new framework allowed us to avoid regularizing the continuum rheology while benefiting from the efficiency of nonsmooth optimization solvers, mainly leveraged by DEM methods so far. Our numerical results were successfully compared to analytic solutions on model problems, such as the silo discharge, and we retrieved qualitative flow features commonly observed in reported experiments of the literature. This work, published at the Journal of Non Newtonian Fluid Mechanics [24], has been extended the approach to account for flows with a varying density, leveraging the Material Point Method to discretize the Drucker Prager yield criterion without linearization. We have also included the handling of anisotropic flow, as well as the coupling of the flow with rigid bodies. These extensions led to a publication at ACM SIGGRAPH 2016 [23].

6.11. Robust Model Predictive Control for biped walking motion generation

Participants: Pierre-Brice Wieber, Diana Serra, Alexander Sherikov, Dimitar Dimitrov.

One of the main sources of nonlinearity in the Newton and Euler equations of motion of biped walking robots lie in the vertical motion of the Center of Mass. We proposed last year an approach that considers this nonlinearity as an uncertainty, in what would else be a linear system. We proposed then to use a robust linear MPC approach accordingly. The use of a linear approach allows fast computations to generate walking motions online. This year, we further developed this approach, by adapting the bounds on the uncertainty at each iteration of a Newton scheme, when solving the original nonlinear problem [35]. By using a robust approach within a Newton scheme, every iteration can be ensured to satisfy all dynamic constraints, so that we can limit the number iterations depending on the available computing power and always obtain a feasible solution. We also developed this year an application of this MPC approach to cases of collaborative carrying of heavy objects with a human partner [32].

6.12. Lexicographic Model Predictive Control for collision avoidance in dynamic environments

Participants: Pierre-Brice Wieber, Nestor Alonso Bohorquez Dorante, Alexander Sherikov, Dimitar Dimitrov.

Collision avoidance may not always be feasible in dynamic environments, when new obstacles can appear too late and move too fast with respect to the dynamic limitations of the system. A typical situation is with a biped robot walking in a compact and uncooperative crowd, with limited field of view. This year, we have investigated and compared 3 different relaxations of the collision avoidance constraint in this setting [33]. In the first case, collisions are accepted if the robot first comes to a stop, what corresponds to standard ISO norms for the safety of robots. In the second case, collisions are actively minimised by the robot, what gives significantly better results. In the third case, for the sake of completeness, the robot is allowed to fall in order to further avoid collisions. All three options were implemented with different formulations of lexicographic relaxation of the constraints in a standard MPC scheme for biped walking motion generation. This work raises important issues regarding safety norms for robots in human environments and how they are implemented.

6.13. Lexicographic Programming

Participants: Pierre-Brice Wieber, Alexander Sherikov, Dimitar Dimitrov, Adrien Escande.

Lexicographic Programming has proved to be a very valuable tool in the last few years for relaxing selectively various constraints and objectives in the control of complex systems such as biped humanoid robots. A major difficulty however is that solutions to such problems very often lie at singular points, making the convergence of standard Newton schemes difficult. We have shown this year how a trust region with filter method can help improve convergence, at least in simple situations [40].

COMMANDS Project-Team

7. New Results

7.1. Optimal control of ordinary and partial differential equations

7.1.1. On the Design of Optimal Health Insurance Contracts under Ex Post Moral Hazard

Participant: Pierre Martinon.

With Pierre Picard and Anasuya Raj, Ecole Polytechnique.
We analyze in [27] the design of optimal medical insurance under ex post moral hazard, i.e., when illness severity cannot be observed by insurers and policyholders decide on their health expenditures. We characterize the trade-o§ between ex ante risk sharing and ex post incentive compatibility, in an optimal revelation mechanism under hidden information and risk aversion. We establish that the optimal contract provides partial insurance at the margin, with a deductible when insurersí rates are a§ected by a positive loading, and that it may also include an upper limit on coverage. We show that the potential to audit the health state leads to an upper limit on out-of-pocket expenses.

7.1.2. Optimal control of infinite dimensional bilinear systems: application to the heat and wave equations

Participants: J. Frédéric Bonnans, Axel Kröner.

With Soledad Aronna, FGV, Rio de Janeiro. In this paper [13] we consider second order optimality conditions for a bilinear optimal control problem governed by a strongly continuous semigroup operator, the control entering linearly in the cost function. We derive first and second order optimality conditions, taking advantage of the Goh transform. We then apply the results to the heat and wave equations.

7.1.3. Optimal control of PDEs in a complex space setting; application to the Schrödinger equation

Participants: J. Frédéric Bonnans, Axel Kröner.

With Soledad Aronna, FGV, Rio de Janeiro. This paper [22] presents some optimality conditions for abstract optimization problems over complex spaces. We then apply these results to optimal control problems with a semigroup structure. As an application we detail the case when the state equation is the Schrödinger one, with pointwise constraints on the "bilinear'" control. We derive first and second order optimality conditions and address in particular the case that the control enters the state equation and cost function linearly.

7.1.4. Approximation and reduction of optimal control problems in infinite dimension

Participant: Axel Kröner.

With Michael D. Chekroun, UCLA) and H. Liu, Virginia Tech. Nonlinear optimal control problems in infinite dimensions are considered for which we establish approximation theorems and reduction procedures. Approximation theorems and reduction procedures are available in the literature. The originality of our approach relies on a combination of Galerkin approximation techniques with reduction techniques based on finite-horizon parameterizing manifolds. The numerical approximation of the control in a feedback form based on Hamilton-Jacobi-Equation become also affordable within this approach. The approach is applied to optimal control problems of delay differential equations and nonlinear parabolic equations.

7.2. Stochastic control, electricity production and planning

7.2.1. MIDAS: A Mixed Integer Dynamic Approximation Scheme

Participant: J. Frédéric Bonnans.

With Andy Philpott and Faisal Wahid, U. Auckland. Mixed Integer Dynamic Approximation Scheme (MIDAS) [23] is a new sampling-based algorithm for solving finite-horizon stochastic dynamic programs with monotonic Bellman functions. MIDAS approximates these value functions using step functions, leading to stage problems that are mixed integer programs. We provide a general description of MIDAS, and prove its almost-sure convergence to an epsilon-optimal policy when the Bellman functions are known to be continuous, and the sampling process satisfies standard assumptions.

7.2.2. Long term aging : an adaptative weights dynamic programming algorithm

Participants: J. Frédéric Bonnans, Benjamin Heymann, Pierre Martinon.

We introduce [26] a class of optimal control problems with periodic data. A state variable that we call the age of the system represents the negative impact of the operations on the system qualities over time: other things being equal, older systems have higher operating costs. Many industrial problems relate to this class. If we envision to perform an optimization over a large number of periods, there is a tradeoff between minimizing repeatedly the one-period criterion in a short sighted way and taking into account the impact of the decision on the aging speed (which modifies the minimal one period criterion). In general, because the aging process is slow, short term optimization strategies-such as one period sliding horizon strategies-either neglect it or use rule-of-thumb penalization terms in the criterion, which leads to suboptimal solutions. On the other hand, for most applications it is unrealistic to envision a brute-force numerical resolution by dynamic programming of the long term problem because of the computation burden. We introduce a two-scale method to reduce this computation burden. The method relies on Lagrangian duality and some monotony properties. We expose the theoretical foundations of the method and discuss some practical aspects: approximation errors, asymptotic estimation, computation burden, possible extensions, etc. Since our initial motivation was the difficulty to take long term battery aging in Energy Management Systems into account, we implement the method on a toy long term microgrid energy management problem.

7.2.3. Continuous Optimal Control Approaches to Microgrid Energy Management

Participants: J. Frédéric Bonnans, Benjamin Heymann, Pierre Martinon.

With Francisco Silva XLIM, U. Limoges, Fernando Lanas and Guillermo Jimenez, U. Chile.

We propose in [18] a novel method for the microgrid energy management problem by introducing a continuous-time, rolling horizon formulation. The energy management problem is formulated as a deterministic optimal control problem (OCP). We solve (OCP) with two classical approaches: the direct method [1], and Bellman's Dynamic Programming Principle (DPP) [2]. In both cases we use the optimal control toolbox BOCOP [3] for the numerical simulations. For the DPP approach we implement a semi-Lagrangian scheme [4] adapted to handle the optimization of switching times for the on/off modes of the diesel generator. The DPP approach allows for an accurate modeling and is computationally cheap. It finds the global optimum in less than 3 seconds, a CPU time similar to the Mixed Integer Linear Programming (MILP) approach used in [5]. We achieve this performance by introducing a trick based on the Pontryagin Maximum Principle (PMP). The trick increases the computation speed by several orders and also improves the precision of the solution. For validation purposes, simulation are performed using datasets from an actual isolated microgrid located in northern Chile. Results show that DPP method is very well suited for this type of problem when compared with the MILP approach.

7.2.4. A Stochastic Continuous Time Model for Microgrid Energy Management

Participants: J. Frédéric Bonnans, Benjamin Heymann.

With Francisco Silva XLIM U. Limoges, Guillermo Jimenez, U. Chile.

We propose in [20] a novel stochastic control formulation for the microgrid energy management problem and extend previous works on continuous time rolling horizon strategy to uncertain demand. We modelize the demand dynamics with a stochastic differential equation. We decompose this dynamics into three terms: an average drift, a time-dependent mean-reversion term and a Brownian noise. We use BOCOPHJB for the numerical simulations. This optimal control toolbox implements a semi-Lagrangian scheme and handle the optimization of switching times required for the discrete on/off modes of the diesel generator. The scheme allows for an accurate modelling and is computationally cheap as long as the state dimension is small. As described in previous works, we use a trick to reduce the search of the optimal control values to six points. This increases the computation speed by several orders. We compare this new formulation with the deterministic control approach using data from an isolated microgrid located in northern Chile.

7.2.5. Mechanism Design and Auctions for Electricity Network

Participant: Benjamin Heymann.

With Alejandro Jofré, CMM - Center for Mathematical Modeling, U. Chile, Santiago. We present in [25] some key aspects of wholesale electricity markets modeling and more specifically focus our attention on auctions and mechanism design. Some of the results arising from those models are the computation of an optimal allocation for the Independent System Operator, the study of the equilibria (existence and unicity in particular) and the design of mechanisms to increase the social surplus. From a more general perspective, this field of research provides clues to discuss how wholesale electricity market should be regulated. We start with a general introduction and then present some results the authors obtained recently. We also briefly expose some undergoing related work. As an illustrative example, a section is devoted to the computation of the Independent System Operator response function for a symmetric binodal setting with piece-wise linear production cost functions.

7.2.6. Mechanism design and allocation algorithms for network markets with piece-wise linear costs and externalities

Participant: Benjamin Heymann.

With Alejandro Jofré, CMM - Center for Mathematical Modeling, U. Chile, Santiago. In [24], motivated by market power in electricity market, we introduce a mechanism design for simplified markets of two agents with linear production cost functions. In standard procurement auctions, the market power resulting from the quadratic transmission losses allow the producers to bid above their true value (i.e. production cost). The mechanism proposed in the previous paper reduces the producers margin to the society benefit. We extend those results to a more general market made of a finite number of agents with piecewise linear cost functions, which make the problem more difficult, but at the same time more realistic. We show that the methodology works for a large class of externalities. We also provide two algorithms to solve the principal allocation problem.

7.2.7. Variational analysis for options with stochastic volatility and multiple factors

Participants: J. Frédéric Bonnans, Axel Kröner.

In this ongoing work we discuss the variational analysis for stochastic volatility models with correlation and their applications for the pricing equations for European options is discussed. The considered framework is based on weigthed Sobolev spaces. Furthermore, to verify continuity of the rate term in the pricing equation an approach based on commutator analysis is developed.

DISCO Project-Team

5. New Results

5.1. Characterizing the Codimension of Zero Singularities for Time-Delay Systems: A Link with Vandermonde and Birkhoff Incidence Matrices

Participants: Islam Boussaada, Silviu-Iulian Niculescu.

The analysis of time-delay systems mainly relies on detecting and understanding the spectral values bifurcations when crossing the imaginary axis. We have dealed with the zero singularity, essentially when the zero spectral value is multiple. The simplest case in such a configuration is characterized by an algebraic multiplicity two and a geometric multiplicity one, known as the Bogdanov-Takens singularity. Moreover, in some cases the codimension of the zero spectral value exceeds the number of the coupled scalar-differential equations. Nevertheless, to the best of the author's knowledge, the bounds of such a multiplicity have not been deeply investigated in the literature. It is worth mentioning that the knowledge of such an information is crucial for nonlinear analysis purposes since the dimension of the projected state on the center manifold is none other than the sum of the dimensions of the generalized eigenspaces associated with spectral values with zero real parts. Motivated by a control-oriented problems, we have provided an answer to this question for time-delay systems, taking into account the parameters' algebraic constraints that may occur in applications. We emphasize the link between such a problem and the incidence matrices associated with the Birkhoff interpolation problem. In this context, symbolic algorithms for LU-factorization for functional confluent Vandermonde as well as some classes of bivariate functional Birkhoff matrices are also proposed [11].

5.2. Tracking the Algebraic Multiplicity of Crossing Imaginary Roots for Generic Quasipolynomials: A Vandermonde-Based Approach

Participants: Islam Boussaada, Silviu-Iulian Niculescu.

A standard approach in analyzing dynamical systems consists in identifying and understanding the eigenvalues bifurcations when crossing the imaginary axis. Efficient methods for crossing imaginary roots identification exist. However, to the best of the author's knowledge, the multiplicity of such roots was not deeply investigated. We have emphasized [12] that the multiplicity of the zero spectral value can exceed the number of the coupled scalar delay-differential equations and a constructive approach Vandermonde-based allowing to an adaptive bound for such a multiplicity is provided. Namely, it is shown that the zero spectral value multiplicity depends on the system structure (number of delays and number of non zero coefficients of the associated quasipolynomial) rather than the degree of the associated quasipolynomial. We have extended the constructive approach in investigating the multiplicity of crossing imaginary roots $j\omega$ where $\omega \neq 0$ and establishes a link with a new class of functional confluent Vandermonde matrices. A symbolic algorithm for computing the LU-factorization for such matrices is provided. As a byproduct of the proposed approach, a bound sharper than the Polya-Szegö generic bound arising from the principle argument is established.

5.3. Coprimeness of fractional representations

Participants: Catherine Bonnet, Le Ha Vy Nguyen, Yutaka Yamamoto [Kyoto Univ].

Coprimeness of a fractional representation plays various crucial roles in many different contexts, for example, stabilization of a given plant, minimality of a state space representation, etc. It should be noted however that coprimeness depends crucially on the choice of a ring (or algebra) where such a representation is taken, which reflects the choice of a plant, and particular problems that one studies. Such relationships are particularly delicate and interesting when dealing with infinite-dimensional systems. We have disucssed various coprimeness issues for different rings, typically for H_∞ and pseudorational transfer functions. The former is related to H_∞-stabilizability, and the latter to controllability of behaviors. We have also given some intricate examples where a seemingly non-coprime factorization indeed turns out to be a coprime factorization over H_∞ [28], [29].

5.4. Output-feddback control design for time-delay systems

Participants: Catherine Bonnet, Caetano Cardeliquio, Matheus Souza [FEEC-UNICAMP], André Fioravanti [FEM-UNICAMP].

We presented new results on H_∞-control synthesis, via output-feedback, for time-delay linear systems. We extend the use of a finite order LTI system, called comparison system, to design a controller which depends not only on the output at the present time and maximum delay, but also on an arbitrary number of values between those. This approach allows us to increase the maximum stable delay without requiring any additional information.

5.5. Backstepping control design through the introduction of delays

Participants: Frederic Mazenc, Michael Malisoff [LSU], Jerome Weston [LSU].

We provided new backstepping results for time-varying systems with input delays. The results were obtained by the introduction of constant 'artificial' pointwise delays in the input. Thus they are significantly different from backstepping results for systems with delay in the input as presented in previous contributions.

I) The novelty of the contribution in [18] is in the bounds on the controls, and the facts that (i) one does not need to compute any Lie derivatives to apply the proposed controls, (ii) the controls have no distributed terms, and (iii) no differentiability conditions on the available controls for the subsystems are needed. The latter aspect is of paramount importance from an applied point of view.

II) In [43], we extended [18]. We provided new globally stabilizing backstepping controls for single input systems in a partially linear form. Instead of measuring the full state, the feedbacks use current and several time lagged values of a function of the state of the nonlinear subsystem (and have no distributed terms). We also allowed input delays. This improves on [18], since we allowed an arbitrary number of integrators whereas [18] is limited to one integrator.

5.6. Switched Nonlinear Systems

Participants: Frederic Mazenc, Yue-E Wang [Shaanxi Normal University], Xi-Ming Sun [Dalian University of Technology].

We considered in [26] a class of nonlinear time-varying switched control systems for which stabilizing feedbacks are available. We analyzed the effect of the presence of a delay in the input of switched nonlinear systems with an external disturbance. By contrast with most of the contributions available in the literature, we did not assume that all the subsystems of the switched system we consider are stable when the delay is present. Through a Lyapunov approach, we derived sufficient conditions in terms of size of the delay, ensuring the global exponential stability of the switched system. Moreover, under appropriate conditions, the input-to-state stability of the system with respect to an external disturbance was established.

5.7. Studies of systems with long delays

Participants: Frederic Mazenc, Michael Malisoff [LSU], Emilia Fridman [Tel-Aviv University].

We solved several problems of observer and control designs pertaining to the fundamental (and difficult) case where a delay in the input is too long for being neglected.

I) We considered in [17] the problem of stabilizing a linear continuous-time system with discrete-time measurements and a sampled input with a pointwise constant delay. In a first part, we designed a continuous-discrete observer which converges when the maximum time interval between two consecutive measurements is sufficiently small. In a second part, we constructed a dynamic output feedback by using a technique which is strongly reminiscent of the so called 'reduction model approach'. It stabilizes the system when the maximal time between two consecutive sampling instants is sufficiently small. No limitation on the size of the delay was imposed and an ISS property with respect to additive disturbances was established.

II) We solved stabilization problems for linear time-varying systems under input delays. We showed how changes of coordinates lead to systems with time invariant drifts, which are covered by the reduction model method and which lead to the problem of stabilizing a time-varying system without delay. For continuous-time periodic systems, we used Floquet's theory to find the changes of coordinates. We also proved an analogue for discrete time systems, through an original discrete-time extension of Floquet's theory [19].

III) In [21] and [42], we proposed a prediction based stabilization approach for a general class of nonlinear time-varying systems with pointwise delay in the input. It is based on a recent new prediction strategy, which makes it possible to circumvent the problem of constructing and estimating distributed terms in the expression for the stabilizing control laws. We observed that our result applies in cases where other recent results do not, including notably the case where a time-varying delay is present.

5.8. Extension of the Razumikhin's theorem

Participants: Frederic Mazenc, Michael Malisoff [LSU].

The Razumikhin's Theorem is a major extension of the Lypunov function theory, making possible to establish the global asymptotic stability of nonlinear systems with delays. It is especially efficient when the delays are time-varying. We provide in [41] an extension of this theorem for continuous-time time-varying systems with time-varying delays. Our result uses a novel 'strictification' technique for converting a nonstrict Lyapunov function into a strict one. Our examples show how our method can sometimes allow broader classes of allowable delays than the results in the literature.

5.9. Observer design for nonlinear systems

Participant: Ali Zemouche.

A new high-gain observer design method with lower gain compared to the standard high-gain observer was proposed. This new observer, called "HG/LMI" observer is obtained by combining the standard high-gain methodology with the LPVLMI-based technique. Through analytical developments, it is shown how the new observer provides a lower gain. A numerical example was used to illustrate the performance of the new "HG/LMI" observer. The aim of this research is the application of this new observer design to estimate some vehicle variables in autonomous vehicle applications.

5.10. Set invariance for discrete-time delay systems

Participants: Sorin Olaru, Mohammed Laraba [L2S], Silviu Niculescu, Franco Blanchini [Univ. Udine, Italy], Stefano Miani [Univ. Udine, Italy].

The existence of positively invariant sets for linear delay-difference equations was pursued in [15]. We made a survey effort and presented in a unified framework all known necessary and/or sufficient conditions for the existence of invariant sets with respect to dynamical systems described by linear discrete time-delay difference equations (dDDEs). Secondly, we address the construction of invariant sets in the original state space (also called D-invariant sets) by exploiting the forward mappings. The notion of D-invariance is appealing since it provides a region of attraction, which is difficult to obtain for delay systems without taking into account the delayed states in some appropriate extended state space model. The paper contains a sufficient condition for the existence of ellipsoidal D-contractive sets for dDDEs, and a necessary and sufficient condition for the existence of D-invariant sets in relation to linear time-varying dDDE stability. Another contribution is the clarification of the relationship between convexity (convex hull operation) and D-invariance of linear dDDEs. In short, it is shown that the convex hull of the union of two or more D-invariant sets is not necessarily D-invariant, while the convex hull of a non-convex D-invariant set is D-invariant. Positive invariance is an essential concept in control theory, with applications to constrained dynam-ical systems analysis, uncertainty handling as well as related control design problems. It serves as a basic tool in many topics, such as model predictive control, fault tolerant control and reference governor design. Furthermore, there exists a close link between classical stability theory and positive invariant sets. It is worth mentioning that, in Lyapunov theory, invariance is implicitly described.

5.11. Interpolation-based design for constrained dynamical systems

Participants: Sorin Olaru, Nam Nguyen [IFP, France], Per Olof Gutman [Technion, Israel].

A technique is presented in [49] leading to an explicit state feedback solution to the regulation problem for uncertain and/or time-varying linear discrete-time systems with state and control constraints. A piecewise affine control law is provided which not only guarantees recursive feasibility and robust asymptotic stability, but is also optimal for a region of the state space containing the origin.

5.12. Inverse optimality results for constrained control

Participants: Sorin Olaru, Ngoc Anh Nguyen [L2S], Pedro Rodriguez [L2S], Morten Hovd [NTNU Trondheim, Norway], Ioan Necoara [Univ. Politehnica Bucharest, Romania].

Parametric convex programming has received a lot of attention, since it has many applications in chemical engineering, control engineering, signal processing , etc. Further, inverse optimality plays an important role in many contexts, e.g., image processing, motion planning. In this context we introduced [10] a constructive solution of the inverse optimality problem for the class of continuous piecewise affine functions. The main idea is based on the convex lifting concept. Accordingly, an algorithm to construct convex liftings of a given convexly liftable partition have been put forward. Continuous piecewise affine function defined over a polytopic partition of the state space are known to be obtained as the solution of a parametric linear/quadratic programming problem. Regarding linear model predictive control, is shown that any continuous piecewise affine control law can be obtained via a linear optimal control problem with the control horizon at most equal to 2 prediction steps.

5.13. Robustness and fragility of Piecewise affine control laws

Participants: Sorin Olaru, Ngoc Anh Nguyen [L2S], Pedro Rodriguez [L2S], Morten Hovd [NTNU Trondheim, Norway], Georges Bitsoris [Univ. Patras, Greece].

We focus in [9]on the robustness and fragility problem for piecewise affine (PWA) control laws for discrete-time linear system dynamics in the presence of parametric uncertainty of the state space model. A generic geometrical approach will be used to obtain robustness/fragility margins with respect to the positive invariance properties. For PWA control laws defined over a bounded region in the state space, it is shown that these margins can be described in terms of polyhedral sets in parameter space. The methodology is further extended to the fragility problem with respect to the partition defining the controller. Finally, several computational aspects are presented regarding the transformation from the theoretical formulations to explicit representations (vertex/halfspace representation of polytopes) of these sets.

5.14. Distributed robust model predictive control

Participants: Sorin Olaru, Alexandra Grancharova [Technical University of Sofia, Bulgaria].

We presented in a suboptimal approach to distributed closed-loop min-max MPC for uncertain systems consisting of polytopic subsystems with coupled dynamics subject to both state and input constraints. The approach applies the dynamic dual decomposition method and reformulates the original centralized min-max MPC problem into a distributed optimization problem. The suggested approach was illustrated on a simulation example of an uncertain system consisting of two interconnected polytopic subsystems.

5.15. Algebraic Analysis Approach to Linear Functional Systems

Participants: Guillaume Sandou, Mohamed Lotfi Derouiche [Ecole nationale d'Ingénieurs de Tunis], Soufiene Bouallegue [Ecole nationale d'Ingénieurs de Tunis], Joseph Haggège Derouiche [Ecole nationale d'Ingénieurs de Tunis].

In this study, a new Model Predictive Controller (MPC) parameters tuning strategy is proposed using a LabVIEW-based perturbed Particle Swarm Optimization (pPSO). This original LabVIEW implementation of this metaheuristic algorithm is firstly validated on some test functions in order to show its efficiency and validity. The optimization results are compared with the standard PSO approach. The parameters tuning problem, i.e. the weighting factors on the output error and input increments of the MPC algorithm, is then formulated and systematically solved, using the proposed LabVIEW pPSA algorithm. The case of a Magnetic Levitation (MAGLEV) system is investigated to illustrate the robustness and superiority of the proposed pPSO-based tuning MPC approach. All obtained simulation results, as well as the statistical analysis tests for the formulated control problem with and without constraints, are discussed and compared with the Genetic Algorithm Optimization (GAO)-based technique in order to improve the effectiveness of the proposed pPSA-based MPC tuning methodology derouiche:hal-01347041.

5.16. Attitude dynamics, control and observation

Participants: Frederic Mazenc, Maruthi Akella [Univ of Texas], Sunpil Yang [Univ of Texas].

In [27], we addressed the rigid-body attitude tracking problem in the absence of angular velocity measurements. To achieve proportional-derivative feedback control, an angular velocity observer with global exponential convergence was designed based on the Immersion and Invariance (I&I) method. A dynamic scaling factor was introduced to circumvent the integrability condition typically arising in I&I design. Unlike the existing I&I observer for this problem, the estimated angular velocity is defined using a rotation matrix of the current quaternion state to avoid use of an additional filter for the angular velocity estimate. As a result, stability analysis became less complex and the observer structure was further simplified by efficient handling of the Coriolis effect in the observer error dynamics. In the case where proportional-derivative control is combined with the observer, asymptotic convergence of tracking errors was proved while establishing a separation property. Numerical simulations were provided to demonstrate the performance of the proposed observer and the output feedback controller.

5.17. Estimation for vehicle application

Participants: Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Gridsada Phanomchoeng [Chulalongkorn University, Thailand].

A new LMI (Linear Matrix Inequality) design technique is developed to address the problem of circle criterion based $\mathcal{H}_\infty$ observer design for nonlinear systems. The developed technique applies to both locally Lipschitz as well as monotonic nonlinear systems, and allows for nonlinear functions in both the process dynamics and output equations. The LMI design condition obtained is less conservative than all previous results proposed in literature for these classes of nonlinear systems. By judicious use of a modified Young's relation, additional degrees of freedom are included in the observer design. These additional decision variables enable improvements in the feasibility of the obtained LMI. Several recent results in literature are shown to be particular cases of the more general observer design methodology developed in this paper. Illustrative examples are used to show the effectiveness of the proposed methodology. The application of the method to slip angle estimation in automotive applications is discussed and experimental results are presented. This application was the main motivation of this work.

5.18. Observer-based stabilization for lateral vehicle control

Participants: Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Yan Wang [University of Minneapolis, USA].

Recently, motivated by autonomous vehicle control problem, a robust observer based estimated state feedback control design method for an uncertain dynamical system that can be represented as a LTI system connected with an IQC-type nonlinear uncertainty was developed. Different from existing design methodologies in which a convex semidefinite constraint is obtained at the cost of conservatism and unrealistic assumptions, the design of the robust observer state feedback controller is formulated in this paper as a feasibility problem of a bilinear matrix inequality (BMI) constraint. Unfortunately, the search for a feasible solution of a BMI constraint is a NP hard problem in general. The applicability of the linearization method, such as variable change method or congruence transformation, depends on the specific structure of the problem at hand and cannot be generalized. A new sequential LMI optimization method to search for a feasible solution was established. A vehicle lateral control problem was presented to demonstrate the applicability of the proposed algorithm to a real-world estimated state feedback control design.

5.19. Unified model for low-cost high-performance AC drives: the equivalent flux concept

Participants: Guillaume Sandou, Mohamad Koteich [Renault], Abdelmalek Maloum [Renault], Gilles Duc [CentraleSupélec].

This study presents a unified modeling approach of alternating current (AC) machines for low-cost high-performance drives. The Equivalent Flux concept is introduced. Using this concept, all AC machines can be seen as a non-salient synchronous machine with modified (equivalent) rotor flux. Therefore, complex salient-rotor machines models are simplified, and unified shaft-sensorless AC drives can be sought. For this purpose, a unified observer-based structure for rotor-flux position and speed estimation is proposed. The equivalent flux concept generalizes the existing concepts, such as the extended back-electromotive force, the fictitious flux and the active flux.

5.20. Supervision and rescheduling of a mixed CBTC traffic on a suburban railway line

Participants: Guillaume Sandou, Juliette Pochet [SNCF], Sylvain Baro [SNCF].

Railway companies need to achieve higher capacities on existing infrastructures such as high density suburban mainlines. Communication based train control (CBTC) systems have been widely deployed on dedicated subway lines. However, deployment on shared rail infrastructure, where CBTC and non-CBTC trains run, leads to a mixed positioning and controlling system with different precision levels and restrictions. New performance and complexity issues are to arise. In this study, a method for rescheduling adapted to a CBTC system running in a mixed traffic, is introduced. The proposed method is based on a model predictive control (MPC) approach. In each step, an enhanced genetic algorithm with new mutation mechanisms solves the problem to optimize the cost function. It determines the dwell times and running times of CBTC trains, taking into account the non-CBTC trains planning and fixed-block localization. In addition, reordering can be allowed by modifying the problem constraints. The work is supported by a simulation tool developed by SNCF and adapted to mixed traffic study. The approach is illustrated with a case study based on a part of an East/West line in the Paris region network, proving the ability of the method to find good feasible solutions when delays occur in traffic [46].

5.21. Combined Feedback Linearization and MPC for Wind Turbine Power Tracking

Participants: Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [CentraleSupélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

The problem of controlling a variable-speedvariable-pitch wind turbine in non conventional operating points is addressed.We aim to provide a control architecture for a general active power tracking problem for the entire operating envelope. The presented control enables to cope with system non linearities while handling state and input constraints, and avoiding singular points. Simulations are carried out based on a 600 kW turbine parameters. Montecarlo simulation shows that the proposed controller presents a certain degree of robustness with respect to the system major uncertainties [36].

5.22. Hierarchical Control of a Wind Farm for Wake Interaction Minimization

Participants: Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [CentraleSupélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

The problem of controlling a wind farm for power optimization by minimizing the wake interaction among wind turbines is addressed. We aim to evaluate the real gain in farm power production when the dynamics of the controlled turbines are taken into account. The proposed local control enables the turbines to track the required power references in the whole operating envelope, and under the major uncertainties of the system. Simulations are carried out based on a wind farm of 600 kW turbines and they show the actual benefit of considering the wake effect in the optimization algorithm [54].

5.23. Control of a model of chemostat with delay

Participants: Frederic Mazenc, Michael Malisoff [LSU], Jerome Harmand [INRA].

We provided in [39] a new control design for models of chemostats, under constant substrate input concentrations, using piecewise constant delayed measurements of the substrate concentration. The growth functions can be uncertain and are not necessarily monotone. The dilution rate is the control. We used a new Lyapunov approach to derive conditions on the largest sampling interval and on the delay length to ensure asymptotic stabilization properties of a componentwise positive equilibrium point.

5.24. Mathematical Modelling of Acute Myeloid Leukemia

Participants: Catherine Bonnet, Jean Clairambault [MAMBA project-team], François Delhommeau [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Walid Djema, Emilia Fridman [Tel-Aviv University], Pierre Hirsch [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Frédéric Mazenc.

ALMA project focuses on analysis of healthy and unhealthy blood cell production. Dynamics of cell populations are modeled and mathematically analyzed in order to explain why some pathological disorders may occur. The challenging problem that we are facing is to steadily extend both modelling and analysis aspects to constantly better represent this complex physiological mechanism, which is not yet fully understood. This year, we have progressed on this line [35] and particular emphasis has been placed on a new generation of differential systems, coupled to algebraic equations, modeling abnormal proliferation as observed in acute myeloid leukemia [65]. We have developed, in [34], Lyapunov-like techniques in order to derive global or local exponential stability conditions for that class of differential-difference hematopoietic models. A new model describing the coexistence between ordinary and mutated hematopoietic stem cells was introduced and analyzed in [33]. Above all, this was about giving theoretical conditions to guarantee the survival of healthy cells while eradicating unhealthy ones. Interpretation of mathematical results leads us to provide possibly innovative therapies by combining drugs infusions. By continuing on the path of models coupling healthy and malignant cells, we proposed a framework to investigate the phenomena of tumour dormancy, which goes beyond leukemias, to cover all types of cancer. Finally, in a recent study, we highlighted the role played by growth factors -hormone-like molecules- on the regulation of various biological features involved in hematopoietic mechanisms; that we interpret in the framework of switching systems with distributed delays.

5.25. Ananlysis of Dengue Fever SIR Model with time-varying parameters

Participants: Stefanella Boatto [Univ Feder Rio de Janeiro], Catherine Bonnet, Frédéric Mazenc.

Dengue fever is an infectious viral disease occuring in humans that is prevalent in parts of Central and South America, Africa, India and South-east Asia and which causes 390 millions of infections worldwilde. We have considered here a SIR model of Dengue fever with a periodically time-dependent infection rate. Such a model has been considered by other authors before but we focused here on different aspects such as the existence of a periodic stable orbit and the importance of the phase of the infection rates.

GECO Project-Team

7. New Results

7.1. New results: geometric control

Let us list some new results in sub-Riemannian geometry and hypoelliptic diffusion obtained by GECO's members.

- In [2] we compare different notions of curvature on contact sub-Riemannian manifolds. In particular we introduce canonical curvatures as the coefficients of the sub-Riemannian Jacobi equation. The main result is that all these coefficients are encoded in the asymptotic expansion of the horizontal derivatives of the sub-Riemannian distance. We explicitly compute their expressions in terms of the standard tensors of contact geometry. As an application of these results, we obtain a sub-Riemannian version of the Bonnet-Myers theorem that applies to any contact manifold.
- In [3] we provide the small-time heat kernel asymptotics at the cut locus in three relevant cases: generic low-dimensional Riemannian manifolds, generic 3D contact sub-Riemannian manifolds (close to the starting point) and generic 4D quasi-contact sub-Riemannian manifolds (close to a generic starting point). As a byproduct, we show that, for generic low-dimensional Riemannian manifolds, the only singularities of the exponential map, as a Lagragian map, that can arise along a minimizing geodesic are A_3 and A_5 (in Arnol'd's classification). We show that in the non-generic case, a cornucopia of asymptotics can occur, even for Riemannian surfaces.
- In [5] we study the evolution of the heat and of a free quantum particle (described by the Schrödinger equation) on two-dimensional manifolds endowed with the degenerate Riemannian metric $ds^2 = dx^2 + |x|^{-2\alpha} d\theta^2$, where $x \in \mathbb{R}$, $\theta \in S^1$ and the parameter $\alpha \in \mathbb{R}$. For $\alpha \leq -1$ this metric describes cone-like manifolds (for $\alpha = -1$ it is a flat cone). For $\alpha = 0$ it is a cylinder. For $\alpha \geq 1$ it is a Grushin-like metric. We show that the Laplace-Beltrami operator Δ is essentially self-adjoint if and only if $\alpha \notin (-3, 1)$. In this case the only self-adjoint extension is the Friedrichs extension Δ_F, that does not allow communication through the singular set $\{x = 0\}$ both for the heat and for a quantum particle. For $\alpha \in (-3, -1]$ we show that for the Schrödinger equation only the average on θ of the wave function can cross the singular set, while the solutions of the only Markovian extension of the heat equation (which indeed is Δ_F) cannot. For $\alpha \in (-1, 1)$ we prove that there exists a canonical self-adjoint extension Δ_N, called bridging extension, which is Markovian and allows the complete communication through the singularity (both of the heat and of a quantum particle). Also, we study the stochastic completeness (i.e., conservation of the L^1 norm for the heat equation) of the Markovian extensions Δ_F and Δ_B, proving that Δ_F is stochastically complete at the singularity if and only if $\alpha \leq -1$, while Δ_B is always stochastically complete at the singularity.
- In [6] we study spectral properties of the Laplace–Beltrami operator on two relevant almost-Riemannian manifolds, namely the Grushin structures on the cylinder and on the sphere. As for general almost-Riemannian structures (under certain technical hypothesis), the singular set acts as a barrier for the evolution of the heat and of a quantum particle, although geodesics can cross it. This is a consequence of the self-adjointness of the Laplace–Beltrami operator on each connected component of the manifolds without the singular set. We get explicit descriptions of the spectrum, of the eigenfunctions and their properties. In particular in both cases we get a Weyl law with dominant term $E \log E$. We then study the effect of an Aharonov-Bohm non-apophantic magnetic potential that has a drastic effect on the spectral properties. Other generalized Riemannian structures including conic and anti-conic type manifolds are also studied. In this case, the Aharonov-Bohm magnetic potential may affect the self-adjointness of the Laplace-Beltrami operator.

- Generic singularities of line fields have been studied for lines of principal curvature of embedded surfaces. In [7] we propose an approach to classify generic singularities of general line fields on 2D manifolds. The idea is to identify line fields as bisectors of pairs of vector fields on the manifold, with respect to a given conformal structure. The singularities correspond to the zeros of the vector fields and the genericity is considered with respect to a natural topology in the space of pairs of vector fields. Line fields at generic singularities turn out to be topologically equivalent to the Lemon, Star and Monstar singularities that one finds at umbilical points.
- In [10] we prove that any corank 1 Carnot group of dimension $k+1$ equipped with a left-invariant measure satisfies the measure contraction property $\mathrm{MCP}(K,N)$ if and only if $K \leq 0$ and $N \geq k+3$. This generalizes the well known result by Juillet for the Heisenberg group H^{k+1} to a larger class of structures, which admit non-trivial abnormal minimizing curves. The number $k+3$ coincides with the geodesic dimension of the Carnot group, which we define here for a general metric space. We discuss some of its properties, and its relation with the curvature exponent (the least N such that the $\mathrm{MCP}(0,N)$ is satisfied). We prove that, on a metric measure space, the curvature exponent is always larger than the geodesic dimension which, in turn, is larger than the Hausdorff one. When applied to Carnot groups, our results improve a previous lower bound due to Rifford. As a byproduct, we prove that a Carnot group is ideal if and only if it is fat.
- In [14] we relate some basic constructions of stochastic analysis to differential geometry, via random walk approximations. We consider walks on both Riemannian and sub-Riemannian manifolds in which the steps consist of travel along either geodesics or integral curves associated to orthonormal frames, and we give particular attention to walks where the choice of step is influenced by a volume on the manifold. A primary motivation is to explore how one can pass, in the parabolic scaling limit, from geodesics, orthonormal frames, and/or volumes to diffusions, and hence their infinitesimal generators, on sub-Riemannian manifolds, which is interesting in light of the fact that there is no completely canonical notion of sub-Laplacian on a general sub-Riemannian manifold. However, even in the Riemannian case, this random walk approach illuminates the geometric significance of Ito and Stratonovich stochastic differential equations as well as the role played by the volume.
- By adapting a technique of Molchanov, we obtain in [15] the heat kernel asymptotics at the sub-Riemannian cut locus, when the cut points are reached by a r-dimensional parametric family of optimal geodesics. We apply these results to the bi-Heisenberg group, that is, a nilpotent left-invariant sub-Riemannian structure on $\mathbb{R}^5$ depending on two real parameters α_1 and α_2. We develop some results about its geodesics and heat kernel associated to its sub-Laplacian and we point out some interesting geometric and analytic features appearing when one compares the isotropic ($\alpha_1 = \alpha_2$) and the non-isotropic cases ($\alpha_1 \neq \alpha_2$). In particular, we give the exact structure of the cut locus, and we get the complete small-time asymptotics for its heat kernel.
- The Whitney extension theorem is a classical result in analysis giving a necessary and sufficient condition for a function defined on a closed set to be extendable to the whole space with a given class of regularity. It has been adapted to several settings, among which the one of Carnot groups. However, the target space has generally been assumed to be equal to $\mathbb{R}^d$ for some $d \geq 1$. We focus in [17] on the extendability problem for general ordered pairs (G_1, G_2) (with G_2 non-Abelian). We analyze in particular the case $G_1 = \mathbb{R}$ and characterize the groups G_2 for which the Whitney extension property holds, in terms of a newly introduced notion that we call pliability. Pliability happens to be related to rigidity as defined by Bryant an Hsu. We exploit this relation in order to provide examples of non-pliable Carnot groups, that is, Carnot groups so that the Whitney extension property does not hold. We use geometric control theory results on the accessibility of control affine systems in order to test the pliability of a Carnot group.
- In [19] we study the cut locus of the free, step two Carnot groups G^k with k generators, equipped with their left-invariant Carnot–Carathéodory metric. In particular, we disprove the conjectures on the shape of the cut loci proposed in the literature, by exhibiting sets of cut points $C \subset G^k$ which, for $k \geq 4$, are strictly larger than conjectured ones. Furthermore, we study the relation of the cut locus with the so-called abnormal set. For each $k \geq 4$, we show that, contrarily to the case $k = 2, 3$,

the cut locus always intersects the abnormal set, and there are plenty of abnormal geodesics with finite cut time. Finally, and as a straightforward consequence of our results, we derive an explicit lower bound for the small time heat kernel asymptotics at the points of C. The question whether C coincides with the cut locus for $k \geq 4$ remains open.

We also edited the two volumes [13] and [12], containing some of the lecture notes of the courses given during the IHP triemster on “Geometry, Analysis and Dynamics on sub-Riemannian Manifolds” which we organized in Fall 2014. The second volume also contains a chapter [11] co-authored by members of the team.

7.2. New results: quantum control

- In recent years, several sufficient conditions for the controllability of the Schrödinger equation have been proposed. In [16], we discuss the genericity of these conditions with respect to the variation of the controlled or the uncontrolled potential. In the case where the Schrödinger equation is set on a domain of dimension one, we improve the results in the literature, removing from the previously known genericity results some unnecessary technical assumptions on the regularity of the potentials.

7.3. New results: neurophysiology

In [4] we propose a supervised object recognition method using new global features and inspired by the model of the human primary visual cortex V1 as the semidiscrete roto-translation group $\mathrm{SE}(2,N) = \mathbb{Z}_N \rtimes \mathbb{R}^2$. The proposed technique is based on generalized Fourier descriptors on the latter group, which are invariant to natural geometric transformations (rotations, translations). These descriptors are then used to feed an SVM classifier. We have tested our method against the COIL-100 image database and the ORL face database, and compared it with other techniques based on traditional descriptors, global and local. The obtained results have shown that our approach looks extremely efficient and stable to noise, in presence of which it outperforms the other techniques it has been compared with.

7.4. New results: switched systems

- In [8] we address the exponential stability of a system of transport equations with intermittent damping on a network of $N \geq 2$ circles intersecting at a single point O. The N equations are coupled through a linear mixing of their values at O, described by a matrix M. The activity of the intermittent damping is determined by persistently exciting signals, all belonging to a fixed class. The main result is that, under suitable hypotheses on M and on the rationality of the ratios between the lengths of the circles, such a system is exponentially stable, uniformly with respect to the persistently exciting signals. The proof relies on a representation formula for the solutions of this system, which allows one to track down the effects of the intermittent damping. A similar representation formula is used in [18] to study the relative controllability of linear difference equations with multiple delays in the state. Thanks to such formula, we characterize relative controllability in time T in terms of an algebraic property of the matrix-valued coefficients, which reduces to the usual Kalman controllability criterion in the case of a single delay. Relative controllability is studied for solutions in the set of all functions and in the function spaces L^p and C^k. We also compare the relative controllability of the system for different delays in terms of their rational dependence structure, proving that relative controllability for some delays implies relative controllability for all delays that are “less rationally dependent" than the original ones. Finally, we provide an upper bound on the minimal controllability time for a system depending only on its dimension and on its largest delay.
- In [9] we address the stability of transport systems and wave propagation on general networks with time-varying parameters. We do so by reformulating these systems as non-autonomous difference equations and by providing a suitable representation of their solutions in terms of their initial conditions and some time-dependent matrix coefficients. This enables us to characterize the asymptotic behavior of solutions in terms of such coefficients. In the case of difference equations with arbitrary switching, we obtain a delay-independent generalization of the well-known criterion for autonomous

systems due to Hale and Silkowski. As a consequence, we show that exponential stability of transport systems and wave propagation on networks is robust with respect to variations of the lengths of the edges of the network preserving their rational dependence structure. This leads to our main result: the wave equation on a network with arbitrarily switching damping at external vertices is exponentially stable if and only if the network is a tree and the damping is bounded away from zero at all external vertices but at most one.

I4S Project-Team

7. New Results

7.1. Outdoor InfraRed Thermography

7.1.1. Autonomous software architecture standardized for infrared and environmental SHM : Cloud2IR

Participants: Antoine Crinière, Jean Dumoulin, Laurent Mevel.

Cloud2IR is an autonomous software architecture, allowing multi-sensor connection (i.e. Infrared Thermography), dedicated to the long term monitoring of infrastructures. Past experimentations have shown the need as well as usefulness of such system. The system has been developed in order to cut down software integration time which facilitates the system adaptation to each experiment specificity. That is why we propose a bi-headed architecture. A specialized part, it represents the sensor specific development as well as their drivers and their different fixed configurations. In our case, as infrared camera are slightly different than other kind of sensors, the system implement in addition an RTSP server which can be used to set up the FOV as well as other measurement parameter considerations and a generic part, which can be seen as the data management side. This last part can be seen as the first embryo of a future generic framework dedicated to the data management of local multisensors (DaMaLoS). It is able to aggregate any sensor data, type or size and automatically encapsulate them in various generic data format as HDF5 or cloud data as OGC SWE standard. This whole part is also responsible of the acquisition scenario the local storage management and the network management through SFTP or SOAP for OGC Web services. Cloud2IR has been deployed on field since more than one year at the SenseCity outdoor test bed and several month at the Inria test bed, both located in France. The system aggregates various sensors as infrared camera, a GPS, multiple pyranometers, a weather station and a proprietary access to the SenseCity data viewer.[40][41]

7.1.2. GPU Improved quantitative analysis of Longterm Infrared-Thermography Data

Participants: Antoine Crinière, Jean Dumoulin, Laurent Mevel.

Since the past decade, infrared thermography coupled with inverse models based on 1d thermal quadrupoles have shown their usefulness in civil engineering by first showing their ability to assess the quantitative non destructive testing of concrete repaired by bonded CFRP plate over a wide area (i.e. repaired or reinforced concrete beams). On the other hand early implementations of long terms monitoring methods based on such approach have given their first results over a whole bridge deck. The experimental method, allow us to have the apparent surface temperature field evolution with time for a wide area divided in pixels. Knowing this specificity, the procedure aims to apply an independent model to each pixel in order to retrieve physical properties map. Such treatment can have a high computational cost. We propose various improvement of our procedure based on GPGPU paradigm in order to shorten the computational time. This study will detail an experimental procedure able to assess the long term thermal monitoring of a bridge deck over days and to draw properties maps of the inner structure. [28]

7.1.3. Infrared thermography for cultural heritage monitoring

Participant: Jean Dumoulin.

Radiation theory helps us to introduce infrared thermography. Infrared thermography is first presented in its passive mode and followed by considerations on active mode. Some processing analysis approaches are described. They belong to signal and image processing domain or to heat transfer domain. Illustration of results obtained with such analysis approaches are described on two experiments carried out in quasi laboratory conditions. Then, a case case study of the monitoring of the Viaduct Basento in Potenza (Southern Italy) is presented. Two features make fascinating this case study. The first one regards the fact that Viaduct Basento is probably the most important and visionary architectural work of the famous structural engineer Sergio Musmeci. The second aspect concerns the application, almost unique in the scientific literature, of an integrated diagnosis approaches combining a wide set of electromagnetic sensing technologies combined with advanced civil engineering analysis methodologies and tools.[44] [45] [22] [23]

7.2. Smarts roads and R5G

7.2.1. Positive surface temperature pavement

Participants: Jean Dumoulin, Nicolas Le Touz.

The mobility during winter season in France mainly relies on the use of de-icers, with an amount ranging from two hundreds thousands tons up to two millions tons for the roads only. Besides the economic impact, there are many concerns on their environmental and infrastructure, both on roads and on airports. In such context and in the framework of the R5G (5th Generation Road) project driven by IFSTTAR, investigations were carried out on the way to modify the infrastructure to maintain pavement surface at a temperature above water freezing point. Two distinct approaches, that can could be combined, were selected. The first one consisted in having a heated fluid circulating in a porous layer within an asphalt concrete pavement sample. The second one specifically relied on the use of paraffin phase change materials (PCM) in cement concrete pavement ones. Experiments on enhanced pavement samples were conducted in a climatic chamber to simulate winter conditions for several continuous days, including wind and precipitations, and monitored by infrared thermography. [24]

7.3. Methods for building performance assessment

7.3.1. Building performance assessment

Participants: Jordan Brouns, Jean Dumoulin, Alexandre Nassiopoulos, Nicolas Le Touz.

Accurate building performance assessment is necessary for the design of efficient energy retrofit operations and to foster the development of energy performance contracts. An important barrier however is that simulation tools fail to accurately predict the actual energy consumption. Two methodology are adressed, first combining thermal sensor output and inverse algorithms to determine the key parameters of a multizone thermal model [15] then assessing wall thermal resistance estimation using infrared thermography and microwave coupling [38][34][43]

7.4. System identification

7.4.1. Variance estimation of modal parameters from subspace-based system identification

Participants: Michael Doehler, Laurent Mevel.

This work has been carried out in collaboration with Philippe Mellinger (former PhD student with Dassault Aviation, now CEA).

An important step in the operational modal analysis of a structure is to infer on its dynamic behavior through its modal parameters. When output-only data is available, i.e. measured responses of the structure, frequencies, damping ratios and mode shapes can be identified assuming that ambient sources like wind or traffic excite the system sufficiently. When also input data is available, i.e. signals used to excite the structure, input/output identification algorithms are used. The use of input information usually provides better modal estimates in a desired frequency range. When identifying the modal parameters from noisy measurement data, the information on their uncertainty is most relevant. In this work, new variance computation schemes for modal parameters are developed for four subspace algorithms, including output-only and input/output methods, as well as data-driven and covariance-driven methods. For the input/output methods, the known inputs are considered as realizations of a stochastic process. Based on Monte Carlo validations, the quality of identification, accuracy of variance estimations and sensor noise robustness are discussed. Finally these algorithms are applied on real measured data obtained during vibrations tests of an aircraft. [19] [37]

7.4.2. Bayesian parameter estimation for parameter varying systems using interacting Kalman filters

Participants: Antoine Crinière, Laurent Mevel, Jean Dumoulin.

Method based on the use of Bayesian modal parameter recursive estimation based on a particular Kalman filter algorithm with decoupled distributions for mass and stiffness. Particular Kalman filtering is a combination of two widely used Bayesian estimation methods working together: the particle filter (also called sequential Monte Carlo samplings) and the Kalman filter. Usual system identification techniques for civil and mechanical structures assume the availability of large set of data derived from a stationary quasi steady structure. On the opposite, several scenarios involve time varying structures. For example, due to interaction with aerodynamics in aeronautics, some critical parameter may have to be monitored, for instability monitoring (leading possibly to flutter) of in flight data due to fuel consumption and speed change. This relates to the monitoring of time varying structural parameters such as frequencies and damping ratios. The main idea of a particular Kalman filter is to consider stochastic particles evolving in the parameter space. For each particle, a corresponding linear state is recursively estimated by applying a Kalman filter to the mechanical system, whose modal parameters are driven by the evolution of this time-varying particle. In order to provide fast and convincing results for large time varying structure, such as an airplane, the execution time of the method has to be improved. Within the Cloud2sm ADT a GPGPU implementation of the algorithm have been developed, now a post-doctoral position have been obtained to improve the algorithm reliability.[29]

7.4.3. Stability of the Kalman filter for continuous time output error systems

Participant: Qinghua Zhang.

This work has been carried out in collaboration with Boyi Ni (SAP Labs China).

The stability of the Kalman filter is usually ensured by the uniform complete controllability *regarding the process noise* and the uniform complete observability of linear time varying systems. This work studies the case of continuous time *output error* systems, in which the process noise is totally absent. The classical stability analysis assuming the controllability regarding the process noise is thus not applicable. It is shown in this work that the uniform complete observability *alone* is sufficient to ensure the asymptotic stability of the Kalman filter applied to time varying *output error* systems, regardless of the stability of the considered systems themselves. The exponential or polynomial convergence of the Kalman filter is then further analyzed for particular cases of stable or unstable output error systems. The results of this work have been published in [20].

7.4.4. Parameter uncertainties quantification for finite element based subspace fitting approaches

Participants: Guillaume Gautier, Laurent Mevel, Michael Doehler.

This work has been carried out in collaboration with Jean-Mathieu Mencik and Roger Serra (INSA Centre Val de Loire).

We address the issue of quantifying uncertainty bounds when updating the finite element model of a mechanical structure from measurement data. The problem arises as to assess the validity of the parameters identification and the accuracy of the results obtained. A covariance estimation procedure is proposed about the updated parameters of a finite element model, which propagates the data-related covariance to the parameters by considering a first-order sensitivity analysis. In particular, this propagation is performed through each iteration step of the updating minimization problem, by taking into account the covariance between the updated parameters and the data-related quantities. Numerical simulations on a beam show the feasibility and the effectiveness of the method. [31]

7.4.5. Embedded subspace-based modal analysis and uncertainty quantification

Participants: Vincent Le Cam, Michael Doehler, Mathieu Le Pen, Ivan Guéguen, Laurent Mevel.

Operational modal analysis is an important step in many methods for vibration-based structural health monitoring. These methods provide the modal parameters (frequencies, damping ratios and mode shapes) of the structure and can be used for monitoring over time. For a continuous monitoring the excitation of a structure is usually ambient, thus unknown and assumed to be noise. Hence, all estimates from the vibration measurements are realizations of random variables with inherent uncertainty due to unknown excitation, measurement noise and finite data length. Estimating the standard deviation of the modal parameters on the same dataset offers significant information on the accuracy and reliability of the modal parameter estimates. However, computational and memory usage of such algorithms are heavy even on standard PC systems in Matlab, where reasonable computational power is provided. In this work, we examine an implementation of the covariance-driven stochastic subspace identification on the wireless sensor platform PEGASE, where computational power and memory are limited. Special care is taken for computational efficiency and low memory usage for an on-board implementation, where all numerical operations are optimized. The approach is validated from an engineering point of view in all its steps, using simulations and field data from a highway road sign structure. [33]

7.5. Damage diagnosis

7.5.1. Estimation of distributed and lumped ohmic losses in electrical cables

Participants: Nassif Berrabah, Qinghua Zhang.

This work has been carried out in the framework of a CIFRE PhD project in collaboration with EDF R&D.

Cables play an important role in modern engineering systems, from power transmission to data communication. In order to ensure reliable and cost-efficient operations, as well as a high level of performance, efficient tools are needed to assess and monitor cables. Hard faults are well handled by existing techniques, whereas soft fault diagnosis still represents an important challenge for current researches. This work focuses on the detection, localization, and estimation of resistive soft fault in electrical cables from reflectometry measurements. A method for the computation of the distributed resistance profile along the cable under test has been developed. Both experimental and simulation results confirm its effectiveness, as reported in the conference paper [26]. A patent based on this work has been registered at INPI (see Section 10.1.4.1).

7.5.2. Fault detection, isolation and quantification from Gaussian residuals

Participants: Michael Doehler, Laurent Mevel, Qinghua Zhang.

Despite the general acknowledgment in the Fault Detection and Isolation (FDI) literature that FDI are typically accomplished in two steps, namely residual generation and residual evaluation, the second step is by far less studied than the first one. This work investigates the residual evaluation method based on the local approach to change detection and on statistical tests. The local approach has the remarkable ability of transforming quite general residuals with unknown or non Gaussian probability distributions into a standard Gaussian framework, thanks to a central limit theorem. In this work, the ability of the local approach for fault quantification is exhibited, whereas previously it was only presented for fault detection and isolation. The numerical computation of statistical tests in the Gaussian framework is also revisited to improve numerical efficiency. An example of vibration-based structural damage diagnosis is presented to motivate the study and to illustrate the performance of the proposed method. [17]

7.5.3. Performance of damage detection in dependence of sample length and measurement noise

Participants: Saeid Allahdadian, Michael Doehler, Laurent Mevel.

In this work the effects of measuring noise and number of samples is studied on the stochastic subspace damage detection (SSDD) technique. In previous studies, the effect of these practical parameters was examined on simulated measurements from a model of a real structure. In this study, these effects are formulated for the expected damage index evaluated from a Chi-square distributed value. Several theorems that describe the effects are proposed and proved. These theorems are used to develop a guideline to serve the user of the SSDD method to face these effects. [25]

7.5.4. Statistical damage localization with stochastic load vectors

Participants: Md Delwar Hossain Bhuyan, Michael Doehler, Laurent Mevel.

The Stochastic Dynamic Damage Locating Vector (SDDLV) method is an output-only damage localization method based on both a Finite Element (FE) model of the structure and modal parameters estimated from output-only measurements in the damage and reference states of the system. A vector is obtained in the null space of the changes in the transfer matrix computed in both states and then applied as a load vector to the model. The damage location is related to this stress where it is close to zero. In previous works an important theoretical limitation was that the number of modes used in the computation of the transfer function could not be higher than the number of sensors located on the structure. It would be nonetheless desirable not to discard information from the identification procedure. In this work, the SDDLV method has been extended with a joint statistical approach for multiple mode sets, overcoming this restriction on the number of modes. The new approach is validated in a numerical application, where the outcomes for multiple mode sets are compared with a single mode set. From these results, it can be seen that the success rate of finding the correct damage localization is increased when using multiple mode sets instead of a single mode set. [27]

7.5.5. Classification of vibration-based damage localization methods

Participant: Michael Doehler.

This work, issued from the COST Action TU1402, is in collaboration with M.P. Limongelli (Politecnico Milan), E. Chatzi (ETH Zürich), G. Lombaert and E. Reynders (both KU Leuven).

After a brief review of vibration based damage identification methods, three different algorithms for damage identification are applied to the case of the benchmark Z24 bridge. Data-driven as well as model-based methods are discussed, including input-output algorithms for taking into account the effect of environmental and/or operational sources on the variability of damage features. A further class of data-driven methods that use finite element information is finally introduced as a possible future development. [35]

7.5.6. Structural system reliability updating with subspace-based damage detection information

Participant: Michael Doehler.

This work is in collaboration with S. Thöns (DTU).

Damage detection systems and algorithms (DDS and DDA) provide information of the structural system integrity in contrast to e.g. local information by inspections or non-destructive testing techniques. However, the potential of utilizing DDS information for the structural integrity assessment and prognosis is hardly exploited nor treated in scientific literature up to now. In order to utilize the information provided by DDS for the structural performance, usually high computational efforts for the pre-determination of DDS reliability are required. In this work, an approach for the DDS performance modelling is introduced building upon the non-destructive testing reliability which applies to structural systems and DDS containing a strategy to overcome the high computational efforts for the pre-determination of the DDS reliability. This approach takes basis in the subspace-based damage detection method and builds upon mathematical properties of the damage detection algorithm. Computational efficiency is gained by calculating the probability of damage indication directly without necessitating a pre-determination for all damage states. The developed approach is applied to a static, dynamic, deterioration and reliability structural system model, demonstrating the potentials for utilizing DDS for risk reduction. [30]

7.5.7. Structural system model updating based on different sensor types

Participants: Dominique Siegert, Xavier Chapeleau, Ivan Guéguen.

Detecting and quantifying early structural damages using deterministic and probabilistic model updating techniques can be achieved by local information in a form of optical strain measurement. The strategy consists in updating physical parameters associated to damages, such as Young's modulus, in order to minimize the gap between the numerical strain obtained from finite element solves and the strain sensor outputs. Generally, the damage estimation is an ill-posed inverse problem, and hence requires regularization. Herein, three model updating techniques are considered involving different type of regularization: classical Tikhonov regularization, constitutive relation error based updating method and Bayesian approach [21]. This work follows an experimental campaign carried out on a post tensioned concrete beam with the aim of investigating the possibility to detect early warning signs of deterioration based on static and/or dynamic tests. Responses of a beam were measured by an extensive set of instruments consisting of accelerometers, inclinometers, displacement transducers, strain gauges and optical fibers. [18].

MCTAO Project-Team

6. New Results

6.1. Advances in optimal control

6.1.1. Algebraic and geometric techniques in medical resonance imaging

Participants: Bernard Bonnard, Jean-Charles Faugère [EPI PolSys], Alain Jacquemard [Univ. de Bourgogne], Mohab Safey El Din [EPI PolSys], Thibaut Verron [EPI PolSys].

In the framework of the ANR-DFG project Explosys (see Section 8.3) we use computer algebra methods to analyze the controlled Bloch equations, modeling the contrast problem in MRI. The problem boils down to analyzing the so called singular extremals associated to the problem. Thanks to the linear dependance of the problem with respect to the state variables and the relaxation parameters the problem is algebraic and is equivalent to determining equilibrium points and eigenvalues of the linearized system at such points together with the algebraic classification of the surface associated to the switches between bang and singular arcs. Preliminary results are described in ISSAC paper [12] using Grobner basis and stratifications of singularities of determinantal varieties. This work was a part of T. Verron's PhD and is continuing in particular with him (Post doc APO-ENSEEIHT).

6.1.2. Local minima, second order conditions

Participants: Jean-Baptiste Caillau, Zheng Chen, Yacine Chitour [Univ. Paris-Sud], Ariadna Farrés [Univ. Barcelona].

It is well known that the PMP gives necessary conditions for optimality, but curves satisfying this condition may be local minima or critical sadle points. Roughly speaking, the PMP is a first order condition. Higher order conditions give finer necessary conditions (and sufficient in some special cases), but they require differentiability that is not always satisfied when commutations occur. Furthermore, these local conditions cannot distinguish local from global minima. In [4] and [19], we make contributions respectively to extending higher order conditions to non-smooth cases and to exploring local and global minima on an example of interest.

Second order systems whose drift is defined by the gradient of a given potential are considered, and minimization of the L^1-norm of the control is addressed in [4]. An analysis of the extremal flow emphasizes the role of singular trajectories of order two [78], [81]; the case of the two-body potential is treated in detail. In L^1-minimization, regular extremals are associated with bang-bang controls (saturated ocnstraint on the norm); in order to assess their optimality properties, sufficient conditions are given for broken extremals and related to the no-fold conditions of [75]. Two examples of numerical verification of these conditions are proposed on a problem coming from space mechanics.

In another direction, we have been studying the structure of local minima for time minimization in the controlled three-body problem. In [19], several homotopies are systematically used to unfold the structure of these local minimizers, and the resulting singularity of the path associated with the value function is analyzed numerically.

6.1.3. Solving chance-constrained optimal control problems in aerospace engineering via Kernel Density Estimation

Participants: Jean-Baptiste Caillau, Max Cerf [Airbus Industries], Achille Sassi, Emmanuel Trélat [Univ. P. & M. Curie], Hasna Zidani [ENSTA ParisTech].

The goal of [30] is to show how non-parametric statistics can be used to solve chance-constrained optimization and optimal control problems by reformulating them into deterministic ones, focusing on the details of the algorithmic approach. We use the Kernel Density Estimation method to approximate the probability density function of a random variable with unknown distribution, from a relatively small sample. In the paper it is shown how this technique can be applied to a class of chance-constrained optimization problem, focusing on the implementation of the method. In particular, in our examples we analyze a chance-constrained version of the well known problem in aerospace optimal control: the Goddard problem.

6.2. Averaging and filtering for optimal control in Space mechanics

Participants: Jean-Baptiste Caillau, Thierry Dargent, Florentina Nicolau, Jean-Baptiste Pomet, Jérémy Rouot.

Investigating averaging in optimal control for space mechanics with low thrust, or more generally with conservative systems with "small" controls is an ongoing subject in the team. It is also central in the research contract with CNES mentioned in Section 7.1 .

6.2.1. Convergence properties of the Maximum principle

Part of Jérémy Rouot's PhD [2] was devoted to convergence properties in the Hamiltonian system resulting from Pontryagin's Maximum principle when the small parameter representing the ratio between slow and fast velocities tends to zero. The difference with previous work is that we give a clear method to sort fast and slow variables in the adjoint variables, and we provide convergence of these under some conditions. A more complete publication is under preparation.

6.2.2. Approximation by filtering in optimal control and applications

Minimum time control of slow-fast systems is considered. In the case of only one fast angle, averaging techniques are available for such systems. The approach introduced in [54] and [43] is recalled, then extended to time dependent systems by means of a suitable filtering operator. The process relies upon approximating the dynamics by means of sliding windows. The size of these windows is an additional parameter that provides intermediate approximations between averaging over the whole fast angle period and the original dynamics. The method was applied to problems coming from space mechanics, and is exposed in [31].

6.2.3. Averaging with reconstruction of the fast variable

We have been studying a way to modify the initial condition of the average equation in order to approach better (but in the mean) the slow variable while reconstructing asymptotically the fast variable. This follows an idea that was shown to work numerically in [54].

In [32], we give a construction for Cauchy problems. It is lighter than second order averaging, in that oscillating signals and ODEs are not used, and still provides a second order error *in the mean*, together with convergence of the fast variable. This remains to be developed for two-point boundary value problems like in optimal control.

6.3. Fully controlled slender microswimmers

6.3.1. The N-link micro-swimmer

Participants: François Alouges [École Polytechnique], Antonio Desimone [SISSA Trieste], Laetitia Giraldi, Marta Zopello [Univ. di Padova].

We discussed a reduced model to compute the motion of slender swimmers which propel themselves by changing the curvature of their body. Our approach is based on the use of Resistive Force Theory for the evaluation of the viscous forces and torques exerted by the surrounding fluid, and on discretizing the kinematics of the swimmer by representing its body through an articulated chain of N rigid links capable of planar deformations. The resulting system of ODEs, governing the motion of the swimmer, is easy to assemble and to solve, making our reduced model a valuable tool in the design and optimization of bio-inspired artificial microdevices. We prove that the swimmer composed by almost 3 segments is controllable in the whole plane. As a direct result, there exists an optimal swimming strategy to reach a desired configuration in minimum time. Numerical experiments for in the case of the Purcell swimmer suggest that the optimal strategy is periodic, namely a sequence of identical strokes. Our results indicate that this candidate for an optimal stroke, indeed gives a better displacement speed than the classical Purcell stroke.

This is presented in [36] (accepted as a Book chapter in Multi-scale Models in Mechano and Tumor Biology: Modeling, Homogenization and Applications, Lecture Notes in Computational Science and Engineering. June 2016).

6.3.2. *Optimal periodic strokes for the Copepod and Purcell micro-swimmers*

Participants: Piernicola Bettiol [Uni. Bretagne Ouest], Bernard Bonnard, Alice Nolot, Jérémy Rouot.

We have analyzed the problem of optimizing the efficiency of the displacement of two micro swimmers with slender links, namely the following two models: the symmetric micro swimmer introduced by Takagi (see [29]); this is a model to describe the locomotion of the micro crustaceans named copepod, and the historical three link Purcell swimmer. The problems are studied in the framework of optimal control theory and SR geometry vs the standard curvature control point of view. Our contributions are to determine the optimal solutions combining geometric analysis and adapted numerical scheme. In particular the nilpotent models introduced in SR geometry allow to make a neat analysis of the problem of determining optimal strokes with small amplitudes and numerical continuation methods are then applied to compute more general stroke. This approach is completely original in optimal control. Also necessary and sufficient optimality conditions are applied to select the topology of optimal strokes (simple loops) and to determine the optimal solution in both cases. For the references see [17] and [27]. Also note that in collaboration with D. Takagi and M. Chyba this approach is currently at the experimental level at the university of Hawaii using a robot micro swimmer mimicking a copepod, see above. More theoretical issues in relation with SR geometry are investigated in the framework of A. Nolot's starting PhD (started August, 2016). Other publication relating these advances are [25], [26], [11].

6.4. Modelization and Controllability of "Magneto-elastic" Micro-swimmers

Participants: François Alouges [École Polytechnique], Antonio Desimone [SISSA Trieste], Laetitia Giraldi, Pierre Lissy [Univ. Paris Dauphine], Clément Moreau [ENS Cachan and York University], Jean-Baptiste Pomet, Marta Zopello [Univ. di Padova].

It is not realistic for *artificial* micro-swimmers built as micro-robots, to have an actuator at each joint. A possibility is as follows: each link of the swimmer bears is magnetized and the movement is controlled via an exterior magnetic field. These models also bear an internal elastic force, that can be modelled as a torsional spring at each joint and tends to asymptotically restore the straight shape in the absence of other forces.

Control strategies for these models have been proved successful numerically. It can also be proved mathematically via an asymptotic analysis that it is possible to steer the swimmer along a chosen direction with some well chosen oscillating magnetic field, provided some obstruction, like symmetries, are avoided. This is exposed in [23] for a Purcell magnetic swimmer (3 links).

For the smallest magneto-elastic micro-swimmer (2 links), we have been able to prove a strong local controllability result (weaker than STLC) around the straight position of the swimmer, again except for values of the parameters that correspond to symmetries preventing controllability. This is exposed in [8], and a note is under preparation, that shows that STLC is indeed *not* satisfied. This analysis is difficult because the straight position corresponds to the equilibria but is very degenerate from the control point of view.

To avoid this degeneracy, a possibility is to “twist” one of the torsional springs so that the equilibria no longer occur for a straight shape. This is exposed in [34] for a 3-link magnetic microswimmer (local controllability has not been proved for this system without the twist). A local partial controllability result around the equilibrium is proved in that case and a constructive method to find the magnetic field that allows the swimmer to move along a prescribed trajectory is described.

6.5. Sub-Riemannian Geometry and Optimal Transport

Participants: Zeinab Badreddine, André Belotto Da Silva [University of Toronto], Ludovic Rifford.

We have studied the Sard Conjecture and its link with the problem of existence and uniqueness of an optimal transport map for a cost given by the square of a sub-Riemannian distance. Given a totally non-holonomic distribution on a smooth manifold, the Sard Conjecture is concerned with the the size of the set of points that can be reached by singular horizontal paths starting from a same point. In the setting of rank-two distributions in dimension three, the Sard conjecture states that that set should be a subset of the so-called Martinet surface of 2-dimensional Hausdorff measure zero. In [24], A. Belotto da Silva and L. Rifford proved that the conjecture holds in the case where the Martinet surface is smooth. Moreover, they address the case of singular real-analytic Martinet surfaces and show that the result holds true under an assumption of non-transversality of the distribution on the singular set of the Martinet surface. The methods rely on the control of the divergence of vector fields generating the trace of the distribution on the Martinet surface and some techniques of resolution of singularities. In a work in progress, the control on the divergence of this "generating" vector field is the key ingredient used by Z. Badreddine to obtain results of existence and uniqueness of optimal transport map for rank-two distribution in dimension four.

6.6. Geometric Control and Dynamics

Participants: Ayadi Lazrag, Ludovic Rifford, Rafael Ruggiero [PUC-RIO].

Following [77], [57] and [58], we apply techniques from geometric control to the study of perturbations of Hamiltonian flows. In [9], we prove a uniform Franks’ lemma at second order for geodesic flows and apply the result in persistence theory.

NECS Project-Team

7. New Results

7.1. Networked and multi-agent systems: modeling, analysis, and estimation

7.1.1. Modeling of animal groups

Participants: P. Frasca [Contact person], A. Aydogdu [Rutgers University at Camden], C. d'Apice [Univ. Salerno], R. Manzo [Univ. Salerno], W. Saidel [Rutgers University at Camden], B. Piccoli [Rutgers University at Camden].

The paper [13] introduces a mathematical model to study the group dynamics of birds resting on wires. The model is agent-based and postulates attraction-repulsion forces between the interacting birds: the interactions are "topological", in the sense that they involve a given number of neighbors irrespective of their distance. The main properties of the model are investigated by combining rigorous mathematical analysis and simulations. This analysis gives indications about the total length of a group and the inter-animal spacings within it: in particular, the model predicts birds to be more widely spaced near the borders of each group. We compare these insights from the model with new experimental data, derived from the analysis of pictures of pigeons and starlings taken by the team in New Jersey. We have used two different image elaboration protocols to derive the data for the statistical analysis, which allowed us to establish a good agreement with the model and to quantify its main parameters. Our data also seem to indicate potential handedness of the birds: we investigated this issue by analyzing the group organization features and the group dynamics at the arrival of new birds. However, data are still insufficient to draw a definite conclusion on this matter. Finally, arrivals and departures of birds from the group are included in a refined version of the model, by means of suitable stochastic processes.

7.1.2. Cyber-Physical Systems: a control-theoretic approach to privacy and security

Participants: A. Kibangou [Contact person], F. Garin, S. Gracy, H. Nouasse.

Cyber-physical systems are composed of many simple components (agents) with interconnections giving rise to a global complex behaviour. Interesting recent research has been exploring how the graph describing interactions affects control-theoretic properties such as controllability or observability, namely answering the question whether a small group of agents would be able to drive the whole system to a desired state, or to retrieve the state of all agents from the observed local states only. A related problem is observability in the presence of an unknown input, where the input can represent a failure or a malicious attack, aiming at disrupting the normal system functioning while staying undetected. In our work [24], we study linear network systems affected by a single unknown input. The main result is a characterization of input and state observability, namely the conditions under which both the whole network state and the unknown input can be reconstructed from some measured local states. This characterization is in terms of observability of a suitably-defined subsystem, which allows the use of known graphical characterizations of observability of cyber-physical systems, leading to structural results (true for almost all interaction weights) or strong structural results (true for all non-zero interaction weights). Observability is also related to privacy issues. In the ProCyPhyS project, started recently (October 2016), we are studying privacy-preserving properties of cyber-physical systems, by analyzing observability properties of such systems, in order to derive privacy-preserving policies for applications related to smart mobility.

7.1.3. Sensor networks: Multisensor data fusion for attitude estimation

Participants: H. Fourati [Contact person], A. Kibangou, A. Makni, T. Michel, P. Geneves [Tyrex, Inria], N. Layaida [Tyrex, Inria], J. Wu [University of Electronic Science and Technology of China, Chengdu], Z. Zhou [University of Electronic Science and Technology of China, Chengdu], D. Belkhiat [University Ferhat Abbas, Setif, Algeria].

Attitude estimation consists in the determination of rigid body orientation in 3D space (principally in terms of Euler angles, rotation matrix, or quaternion). This research area is a multilevel, multifaceted process involving the automatic association, correlation, estimation, and combination of data and information from several sources. Another interest consists in the fact that redundant and complementary sensor data can be fused and integrated using multisensor fusion techniques to enhance system capability and reliability. Data fusion for attitude estimation is therefore a research area that borrows ideas from diverse fields, such as signal processing, sensor fusion, and estimation theory, where enhancements are involved in point-of-view data authenticity or availability. Data fusion for attitude estimation is motivated by several issues and problems, such as data imperfection, data multimodality, data dimensionality, and processing framework. As a majority of these problems have been identified and heavily investigated, no single data fusion algorithm is capable of addressing all the aforementioned challenges. Consequently, a variety of methods in the literature focuses on a subset of these issues. These concepts and ideas are treated in the book [28], as a response to the great interest and strong activities in the field of multisensor attitude estimation during the last few years, both in theoretical and practical aspects. In the team, we have carried out works related to attitude estimation evaluation for pedestrian navigation purpose. In [18], we focused on two main challenges. The first one concerns the attitude estimation during dynamic cases, in which external acceleration occurs. In order to compensate for such external acceleration, we design a quaternion-based adaptive Kalman filter q-AKF. Precisely, a smart detector is designed to decide whether the body is in static or dynamic case. Then, the covariance matrix of the external acceleration is estimated to tune the filter gain. The second challenge is related to the energy consumption issue of gyroscope. In order to ensure a longer battery life for the Inertial Measurement Units, we study the way to reduce the gyro measurements acquisition by switching on/off the sensor while maintaining an acceptable attitude estimation. The switching policy is based on the designed detector. The efficiency of the proposed scheme is evaluated by means of numerical simulations and experimental tests. In [31], 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. A novel quaternion-based attitude estimator with magnetic, angular rate, and gravity (MARG) sensor arrays is proposed in [20] within the framework of collaboration with Prof. Zhou from University of Electronic Science and Technology of China, Chengdu. A new structure of a fixed-gain complementary filter is designed fusing related sensors. To avoid using iterative algorithms, the accelerometer-based attitude determination is transformed into a linear system. Stable solution to this system is obtained via control theory. With only one matrix multiplication, the solution can be computed. Using the increment of the solution, we design a complementary filter that fuses gyroscope and accelerometer together. The proposed filter is fast, since it is free of iteration. We name the proposed filter the fast complementary filter (FCF). To decrease significant effects of unknown magnetic distortion imposing on the magnetometer, a stepwise filtering architecture is designed. The magnetic output is fused with the estimated gravity from gyroscope and accelerometer using a second complementary filter when there is no significant magnetic distortion. Several experiments are carried out on real hardware to show the performance and some comparisons. Results show that the proposed FCF can reach the accuracy of Kalman filter. It successfully finds a balance between estimation accuracy and time consumption. Compared with iterative methods, the proposed FCF has much less convergence speed. Besides, it is shown that the magnetic distortion would not affect the estimated Euler angles.

7.2. Control design and networked systems

7.2.1. Control design for hydro-electric power-plants

Participants: C. Canudas de Wit [Contact person], S. Gerwig [Feb 2014–Mar 2016], F. Garin, B. Sari [Alstom].

This is the study of collaborative and resilient control of hydro-electric power-plants, in collaboration with Alstom. The goal is to improve performance of a hydro-electric power-plant outside its design operation conditions, by cancellation of oscillations that occur in such an operation range. Indeed, current operation of power-plants requires to operate on a variety of conditions, often different from the ones initially considered when designing the plant. At off-design operation pressure, the hydraulic turbine exhibits a vortex rope below the runner. This vortex generates pressure fluctuations after the turbine and can excite the hydraulic pipes. Indeed the water is compressible and the pipe walls elastic, so the system can oscillate. The goal is to damp these pressure oscillations as they create vibrations in the system and can lead to damages. Our first contribution [23] has been to model the effect of the vortex rope on the hydraulic system as an external perturbation source acting on pipes. The pipes themselves are described with equations taking into account water compressibility and pipe-wall elasticity. The resulting model is nonlinear with hyperbolic functions in the equations (analogous to high-frequency transmission lines), from which we obtain a suitably linearized model. This model can then be used for control design.

7.2.2. Collaborative source seeking

Participants: F. Garin [Contact person], C. Canudas de Wit, R. Fabbiano.

The problem of source localization consists in finding the point or the spatial region from which a quantity of interest is being emitted. We consider collaborative source seeking, where various moving devices, each equipped with a sensor, share information to coordinate their motion towards the source. We focus on the case where information can only be shared locally (with neighbor agents) and where the the agents have no global position information, and only limited relative information (bearing angle of neighbor agents). This setup is relevant when GPS navigation is not available, as in underwater navigation or in cave exploration, and when relative position of neighbors is vision-based, making it easier to measure angles than distances. In [16] we propose and analize a control law, which is able to bring and keep the agents on a circular equispaced formation, and to steer the circular formation towards the source via a gradient-ascent technique; the circular equispaced formation is beneficial to a good approximation of the gradient from local pointwise measurements. This algorithm is different from the ones present in the literature, because it can cope with our above-described restrictive assumptions on the available position information.

7.2.3. Distributed control and game theory: self-optimizing systems

Participants: F. Garin [Contact person], B. Gaujal [POLARIS], S. Durand.

The design of distributed algorithms for a networked control system composed of multiple interacting agents, in order to drive the global system towards a desired optimal functioning, can benefit from tools and algorithms from game theory. This is the motivation of the Ph.D. thesis of Stéphane Durand, a collaboration between POLARIS and NECS teams. The first results of this thesis concern the complexity of a classical algorithm in game theory, the Best Response Algorithm, an iterative algorithm to find a Nash Equilibrium. For potential games, Best Response Algorithm converges in finite time to a pure Nash Equilibrium. The worse-case convergence time is known to be exponential in the number of players, but surprisingly it turns out that on average (over the possible values of the potentials) the complexity is much smaller, only linearly growing, see [27], [26], [22].

7.3. Transportation networks and vehicular systems

7.3.1. Travel time prediction

Participants: A. Kibangou [Contact person], C. Canudas de Wit, H. Fourati, A. Ladino.

One of the regular performance metrics for qualifying the level of congestion in traffic networks is the travel time. Precision in the estimation or measurement of this variable is one of the most desired features for traffic management. The computation of the travel time is regularly performed based on instantaneous information so called instantaneous travel time (ITT), but regularly traffic changes on time and spaces and the computation depends dynamically on the speeds of the system and the notion of dynamic travel time (DTT) is required. Here the computation requires future information of speed so a short term forecast is required. First in [25] we have presented a framework for instantaneous travel time predictions for multiple origins and destinations in a highway. Secondly in [32], a detailed real time application to compute predictions of dynamic travel time (DTT) is presented. Speed measurements describing a spatio-temporal distribution are captured, from there the DTT is constructed. Definitions, computational details and properties in the construction of DTT are provided. DTT is dynamically clustered using a K-means algorithm and then information on the level and the trend of the centroid of the clusters is used to devise predictors computationally simple to be implemented. To take into account lack of information of cluster assignment of the data to be predicted, a fusion strategy based on the best linear unbiased estimator principle is proposed to combine the predictions of each model. The algorithm is deployed in a real time application and the performance is evaluated using real traffic data from the South Ring of the Grenoble city in France.

7.3.2. Urban traffic control

Participants: C. Canudas de Wit [Contact person], F. Garin, P. Grandinetti.

This work deals with optimal or near-optimal operation of traffic lights in an urban area, e.g., a town or a neighborhood. The goal is on-line optimization of traffic lights schedule in real time, so as to take into account variable traffic demands, with the objective of obtaining a better use of the road infrastructure. More precisely, we aim at maximizing total travel distance within the network, while also ensuring good servicing of demands of incoming cars in the network from other areas. The complexity of optimization over a large area is addressed both in the formulation of the optimization problem, with a suitable choice of the traffic model, and in a distributed solution, which not only parallelizes computations, but also respects the geometry of the town, i.e., it is suitable for an implementation in a smart infrastructure where each intersection can compute its optimal traffic lights by local computations combined with exchanges of information with neighbor intersections.

7.3.3. Optimal control of freeway access

Participants: C. Canudas de Wit [Contact person], D. Pisarski.

The work [19] contains Dominik Pisarski's major results which he obtained during the realization of his Ph.D. thesis at Inria-Rhone Alpes. In concerns the problem of optimal control for balancing traffic density in freeway traffic. The control is realized by ramp metering. The balancing of traffic was proposed as a new objective to improve the vehicular flow on freeways and ring-roads. It was demonstrated that the balancing may result in significantly shortened travel delays and reduced pollution. It may also be beneficial for safety and comfort during a travel. For the controller, a novel modular decentralized structure was proposed where each of the modules computes its optimal decision by using local traffic state and supplementary information arriving from the neighboring controllers. For such a structure, the optimal control problem was formulated as a Nash game, where each player (controller's module) optimizes its local subsystem with respect to decisions of the other players. In comparison to the existing solutions, this new approach significantly reduces the computational burden needed for optimal traffic control, allowing for on-line implementation over long freeway segments. In the paper, the proposed control method was tested via numerical examples with the use of Cell Transmission Model. Later, the performance of the designed method was validated by employing a micro-simulator and real traffic data collected from the south ring of Grenoble. The designed distributed controller resulted in 5% reduction of total time spent on the ring road, 18% reduction of total time spent in the on-ramp queues, 2reduction of the average fuel consumption, and 4% reduction of the traffic density.

NON-A Project-Team

7. New Results

7.1. Homogeneity Theory

Homogeneity is one of the tools we develop for finite-time convergence analysis. In 2016 this concept has received various improvements:

- Frequency domain approach to analysis of homogeneous nonlinear systems [85], [46]:

  Analysis of feedback sensitivity functions for implicit Lyapunov function-based control system is developed. The Gang of Four and loop transfer function are considered for practical implementation of the control via frequency domain control design. The effectiveness of this control scheme is demonstrated on an illustrative example of roll control for a vectored thrust aircraft.
- Homogeneous distributed parameter systems [72], [32]:

  A geometric homogeneity is introduced for evolution equations in a Banach space. Scalability property of solutions of homogeneous evolution equations is proven. Some qualitative characteristics of stability of trivial solution are also provided. In particular, finite-time stability of homogeneous evolution equations is studied. Classical theorems on existence and uniqueness of solutions of nonlinear evolution equations are revised. A universal homogeneous feedback control for a finite-time stabilization of linear evolution equation in a Hilbert space is designed using homogeneity concept. The design scheme is demonstrated for distributed finite-time control of heat and wave equations.
- Robustness of Homogenous Systems:
  - [93], [36] The problem of stability robustness with respect to time-varying perturbations of a given frequency spectrum is studied applying homogeneity framework. The notion of finite-time stability over time intervals of finite length, i.e. short-finite-time stability, is introduced and used for that purpose. The results are applied to demonstrate some robustness properties of the three-tank system.
  - The uniform stability notion for a class of nonlinear time-varying systems is studied in [35] using the homogeneity framework. It is assumed that the system is weighted homogeneous considering the time variable as a constant parameter, then several conditions of uniform stability for such a class of systems are formulated. The results are applied to the problem of adaptive estimation for a linear system.
  - Robustness with respect to delays is discussed in [84], [45] for homogeneous systems with negative degree. It is shown that if homogeneous system with negative degree is globally asymptotically stable at the origin in the delay-free case then the system is globally asymptotically stable with respect to a compact set containing the origin independently of delay. The possibility of applying the result for local analysis of stability for not necessary homogeneous systems is analyzed. The theoretical results are supported by numerical examples.
- Finite-time and Fixed-time Control and Estimation:
  - [61], [46] A switched supervisory algorithm is proposed, which ensures fixed-time convergence by commutation of finite-time or exponentially stable homogeneous systems of a special class, and a finite-time convergence to the origin by orchestrating among asymptotically stable systems. A particular attention is paid to the case of exponentially stable systems. Finite-time and fixed-time observation problem of linear multiple input multiple output (MIMO) control systems is studied. The nonlinear dynamic observers , which guarantee convergence of the observer states to the original system state in a finite and a fixed (defined a priori) time, are studied. Algorithms for the observers parameters tuning are also developed.

  - [16] This paper focuses on the design of fixed-time consensus for multiple unicycle-type mobile agents. A distributed switched strategy, based on local information, is proposed to solve the leader-follower consensus problem for multiple nonholonomic agents in chained form. The switching times and the prescribed convergence time are explicitly given regardless of the initial conditions. Simulation results highlight the efficiency of the proposed method.
- Discretization of Homogeneous Systems:
  - [63] Sufficient conditions for the existence and convergence to zero of numeric approximations to solutions of asymptotically stable homogeneous systems are obtained for the explicit and implicit Euler integration schemes. It is shown that the explicit Euler method has certain drawbacks for the global approximation of homogeneous systems with non-zero degrees, whereas the implicit Euler scheme ensures convergence of the approximating solutions to zero.
  - [69] The known results on asymptotic stability of homogeneous differential inclusions with negative homogeneity degrees and their accuracy in the presence of noises and delays are extended to arbitrary homogeneity degrees. Discretization issues are considered, which include explicit and implicit Euler integration schemes. Computer simulation illustrates the theoretical results.
- Multi-Homogeneity and differential inclusions:
  - The notion of homogeneity in the bi-limit from is extended in [21] to local homogeneity and then to homogeneity in the multi-limit. The converse Lyapunov/Chetaev theorems on (homogeneous) system instability are obtained. The problem of oscillation detection for nonlinear systems is addressed. The sufficient conditions of oscillation existence for systems homogeneous in the multi-limit are formulated. The proposed approach estimates the number of oscillating modes and the regions of their location. Efficiency of the technique is demonstrated on several examples.
  - In [94], the notion of geometric homogeneity is extended for differential inclusions. This kind of homogeneity provides the most advanced coordinate-free framework for analysis and synthesis of nonlinear discontinuous systems. The main qualitative properties of continuous homogeneous systems are extended to the discontinuous setting: the equivalence of the global asymptotic stability and the existence of a homogeneous Lyapunov function; the link between finite-time stability and negative degree of homogeneity; the equivalence between attractivity and asymptotic stability are among the proved results.

7.2. Algebraic Technique For Estimation

- Time parameter estimation for a sum of sinusoidal waveform signals [39]:

  A novel algebraic method is proposed to estimate amplitudes, frequencies, and phases of a biased and noisy sum of complex exponential sinusoidal signals. The resulting parameter estimates are given by original closed formulas, constructed as integrals acting as time-varying filters of the noisy measured signal. The proposed algebraic method provides faster and more robust results, compared with usual procedures. Some computer simulations illustrate the efficiency of our method.
- Algebraic estimation via orthogonal polynomials [80]:

  Many important problems in signal processing and control engineering concern the reconstitution of a noisy biased signal. For this issue, we consider the signal written as an orthogonal polynomial series expansion and we provide an algebraic estimation of its coefficients. We specialize in Hermite polynomials. On the other hand, the dynamical system described by the noisy biased signal may be given by an ordinary differential equation associated with classical orthogonal polynomials. The signal may be recovered through the coefficients identification. As an example, we illustrate our algebraic method on the parameter estimation in the case of Hermite polynomials.

- An effective study of the algebraic parameter estimation problem [105]:

  Within the algebraic analysis approach, we first give a general formulation of the algebraic parameter estimation for signals which are defined by ordinary differential equations with polynomial coefficients such as the standard orthogonal polynomials (Chebyshev, Jacobi, Legendre, Laguerre, Hermite, ... polynomials). We then show that the algebraic parameter estimation problem for a truncated expansion of a function into an orthogonal basis of L^2 defined by orthogonal polynomials can be studied similarly. Then, using symbolic computation methods such as Gröbner basis techniques for (noncommutative) polynomial rings, we first show how to compute ordinary differential operators which annihilate a given polynomial and which contain only certain parameters in their coefficients. Then, we explain how to compute the intersection of the annihilator ideals of two polynomials and characterize the ordinary differential operators which annihilate a first polynomial but not a second one. These results are implemented in the NON-A package built upon the OREMODULES software.

7.3. Set-Theoretic Methods of Control, Observer Design and Estimation

- Interval Observers:
  - [19] New design of interval observers for continuous-time systems with discrete-time measurements is proposed. For this purpose new conditions of positivity for linear systems with sampled feedbacks are obtained. A sampled-data stabilizing control is synthesized based on provided interval estimates. Efficiency of the obtained solution is demonstrated on examples.
  - [66] The problem of interval state estimation is studied for systems described by parabolic Partial Differential Equations (PDEs). The proposed solution is based on a finite-element approximation of PDE, with posterior design of an interval observer for the obtained ordinary differential equation. The interval inclusion of the state function of PDE is obtained using the estimates on the error of discretization. The results are illustrated by numerical experiments with an academic example.
  - [18] New interval observers are designed for linear systems with time-varying delays in the case of delayed measurements. Interval observers employ positivity and stability analysis of the estimation error system, which in the case of delayed measurements should be delay-dependent. New delay-dependent conditions of positivity for linear systems with time-varying delays are introduced. Efficiency of the obtained solution is demonstrated on examples.
  - [22] Interval state observers provide an estimate on the set of admissible values of the state vector at each instant of time. Ideally, the size of the evaluated set is proportional to the model uncertainty, thus interval observers generate the state estimates with estimation error bounds, similarly to Kalman filters, but in the deterministic framework. Main tools and techniques for design of interval observers are reviewed in this tutorial for continuous-time, discrete-time and time-delayed systems.
  - [43] investigates the problem of observer design for a general class of linear singular time-delay systems, in which the time delays are involved in the state, the output and the known input (if there exists). The involvement of the delay could be multiple which however is rarely studied in the literature. Sufficient conditions are proposed which guarantees the existence of a Luenberger-like observer for the general system.
  - In [90] an interval observer is proposed for on-line estimation of differentiation errors in some class of high-order differentiators (like a high-gain differentiator, or homogeneous nonlinear differentiator, or super-twisting differentiator). The results are verified and validated on the telescopic link of a robotic arm for forestry applications in which the mentioned approaches are used to estimate the extension velocity while the interval observer gives bounds to this estimation.

- The problem of interval observer design is studied in [87] for a class of linear hybrid systems. Several observers are designed oriented on different conditions of positivity and stability for estimation error dynamics. Efficiency of the proposed approach is demonstrated by computer experiments for academic and bouncing ball systems.
- The problem of estimation of sequestered parasites Plasmodium falciparum in malaria, based on measurements of circulating parasites, is addressed in [60]. It is assumed that all (death, transition, recruitment and infection) rates in the model of a patient are uncertain (just intervals of admissible values are given) and the measurements are subject to a bounded noise, then an interval observer is designed. Stability of the observer can be verified by a solution of LMI. The efficiency of the observer is demonstrated in simulation.

- Observer design:
  - [81] presents a new approach for observer design for a class of nonlinear singular systems which can be transformed into a special normal form. The interest of the proposed form is to facilitate the observer synthesis for the studied nonlinear singular systems. Necessary and sufficient geometrical conditions are deduced in order to guarantee the existence of a diffeomorphism which transforms the studied nonlinear singular systems into the proposed normal form.
  - In [38], we investigate the estimation problem for a class of partially observable nonlinear systems. For the proposed Partial Observer Normal Form (PONF), necessary and sufficient conditions are deduced to guarantee the existence of a change of coordinates which can transform the studied system into the proposed PONF. Examples are provided to illustrate the effectiveness of the proposed results.
  - [71] deals with the problem of finite-time and fixed-time observation of linear multiple input multiple output (MIMO) control systems. The nonlinear dynamic observers , which guarantee convergence of the observer states to the original system state in a finite and a fixed (defined a priori) time, are studied. Algorithms for the observers parameters tuning are also developed. The theoretical results are illustrated by numerical examples.
  - [44] Sliding mode control design for linear systems with incomplete and noisy measurements of the output and additive/multiplicative exogenous disturbances is studied. A linear minimax observer estimating the system's state with minimal worst-case error is designed. An algorithm, generating continuous and discontinuous feedbacks, which steers the state as close as possible to a given sliding hyperplane in finite time, is presented. The optimality (sub-optimality) of the designed feedbacks is proven for the case of bounded noises and additive (multiplicative) disturbances of L_2-class.
  - [37] deals with the design of a robust control for linear systems with external disturbances using a homogeneous differentiator-based observer based on a implicit Lyapunov function approach. Sufficient conditions for stability of the closed-loop system in the presence of external disturbances are obtained and represented by linear matrix inequalities. The parameter tuning for both controller and observer is formulated as a semi-definite programming problem with linear matrix inequalities constraints. Simulation results illustrate the feasibility of the proposed approach and some improvements with respect to the classic linear observer approach.
  - The problem studied in [17] is one of improving the performance of a class of adaptive observer in the presence of exogenous disturbances. The H^∞ gains of both a conventional and the newly proposed sliding-mode adaptive observer are evaluated, to assess the effect of disturbances on the estimation errors. It is shown that if the disturbance is "matched" in the plant equations, then including an additional sliding-mode feedback injection term, dependent on the plant output, improves the accuracy of observation.

  - In [95], we consider the classical reaching problem of sliding mode control design, that is to find a control law which steers the state of a Linear Time-Invariant (LTI) system towards a given hyperplane in a finite time. Since the LTI system is subject to unknown but bounded disturbances we apply the minimax observer which provides the best possible estimate of the system's state. The reaching problem is then solved in observer's state space by constructing a feedback control law. The cases of discontinuous and continuous admissible feedbacks are studied. The theoretical results are illustrated by numerical simulations.
- Estimation and Identification:
  - The problem of output control for linear uncertain system with external perturbations is studied in [77]. It is assumed that the output available for measurements is the higher order derivative of the state only (acceleration for a second order plant), which is also corrupted by noise. Then via series of integration an identification algorithm is proposed for identification of values of all parameters and unknown initial conditions for the state vector. Finally, two control algorithms are developed, adaptive and robust, providing boundedness of trajectories for the system. Efficiency of the obtained solutions is demonstrated by numerical experiments.
  - [24] focuses on the problem of velocity and position estimation. A solution is presented for a class of oscillating systems in which position, velocity and acceleration are zero mean signals. The proposed scheme considers that the dynamic model of the system is unknown. Only noisy acceleration measurements, that may be contaminated by zero mean noise and constant bias, are considered to be available. The proposal uses the periodic nature of the signals obtaining finite-time estimations while tackling integration drift accumulation.
  - In [41], we investigate the problem of simultaneous state and parameter estimation for a class of nonlinear systems which can be transformed into an output depending normal form. A new and simple adaptive observer for such class of systems is presented. Sufficient condition for the existence of the proposed observer is derived. A concrete application is given in order to highlight the effectiveness of the proposed result.
  - In [75], the problem of time-varying parameter identification is studied. To this aim, an identification algorithm is developed in order to identify time-varying parameters in a finite-time. The convergence proofs are based on a notion of finite-time stability over finite intervals of time, i.e. Short-finite-time stability; homogeneity for time-varying systems; and Lyapunov function approach. The algorithm asks for a condition over the regressor term which is related to the classic identifiability condition corresponding to the injectivity of such a term. Simulation results illustrate the feasibility of the proposed algorithm.

7.4. Stability, Stabilization, Synchronization

- Input-to-state stability:
  - Supported by a novel field definition and recent control theory results, a new method to avoid local minima is proposed in [25]. It is formally shown that the system has an attracting equilibrium at the target point, repelling equilibriums in the obstacles centers and saddle points on the borders. Those unstable equilibriums are avoided capitalizing on the established Input-to-State Stability (ISS) property of this multistable system. The proposed modification of the PF method is shown to be effective by simulation for a two variables integrator and then applied to an unicycle-like wheeled mobile robots which is subject to additive input disturbances.
  - [62] Motivated by the problem of phase-locking in droop-controlled inverter-based microgrids with delays, the recently developed theory of input-to-state stability (ISS) for multistable systems is extended to the case of multistable systems with delayed dynamics. Sufficient conditions for ISS of delayed systems are presented using Lyapunov-Razumikhin

functions. It is shown that ISS multistable systems are robust with respect to delays in a feedback. The derived theory is applied to two examples. First, the ISS property is established for the model of a nonlinear pendulum and delay-dependent ro-bustness conditions are derived. Second, it is shown that, under certain assumptions, the problem of phase-locking analysis in droop-controlled inverter-based microgrids with delays can be reduced to the stability investigation of the nonlinear pendulum. For this case, corresponding delay-dependent conditions for asymptotic phase-locking are given.

  - [103] A necessary and sufficient criterion to establish input-to-state stability (ISS) of nonlinear dynamical systems, the dynamics of which are periodic with respect to certain state variables and which possess multiple invariant solutions (equilibria, limit cycles, etc.), is provided. Unlike standard Lyapunov approaches, the condition is relaxed and formulated via a sign-indefinite function with sign-definite derivative, and by taking the system's periodicity explicitly into account. The new result is established by using the framework of cell structure introduced in [24] and it complements the methods developed in [3], [4] for periodic systems. The efficiency of the proposed approach is illustrated via the global analysis of a nonlinear pendulum with constant persistent input.
  - In [53] we revisit the problem of stabilizing a triple integrator using a control that depends on the signs of the state variables. For a more general class of linear systems it is shown that the stabilization by sign feedback is possible, depending on some properties of the system's matrix. The conditions for the stability are established by means of linear matrix inequalities. For the triple integrator, the domain of stability is evaluated. Also, the control law is augmented by a linear feedback and the stability properties for this case, checked. The results are illustrated by numerical experiments for a chain of integrators of third order.

- Stabilization:
  - A solution to the problem of global fixed-time output stabilization of a chain of integrators is proposed in [70]. A nonlinear state feedback and a dynamic observer are designed in order to guarantee both fixed-time estimation and fixed-time control. Robustness with respect to exogenous disturbances and measurement noises is established. The performance of the obtained control and estimation algorithms are illustrated by numeric experiments.
  - In [20], the rate of convergence to the origin for a chain of integrators stabilized by homogeneous feedback is accelerated by a supervisory switching of control parameters. The proposed acceleration algorithm ensures a fixed-time convergence for otherwise exponentially or finite-time stable homogeneous closed-loop systems. Bounded disturbances are taken into account. The results are especially useful in the case of exponentially stable systems widespread in the practice. The proposed switching strategy is illustrated by computer simulation.
  - [33] The problem of robust finite-time stabilization of perturbed multi-input linear system by means of generalized relay feedback is considered. A new control design procedure, which combines convex embedding technique with Implicit Lyapunov Function (ILF) method, is developed. The sufficient conditions for both local and global finite-time stabilization are provided. The issues of practical implementation of the obtained implicit relay feedback are discussed. Our theoretical result is supported by numerical simulation for a Buck converter.
  - [100] contributes to the stability analysis for impulsive dynamical systems based on a vector Lyapunov function and its divergence operator. The new method relies on a 2D time domain representation. The result is illustrated for the exponential stability of linear impulsive systems based on LMIs. The obtained results provide some notions of minimum and maximum dwell-time. Some examples illustrate the feasibility of the proposed approach.

  - The Universal Integral Control, introduced in H.K. Khalil, is revisited in [34] by employing mollifiers instead of a high-gain observer for the differentiation of the output signal. The closed loop system is a classical functional differential equation with distributed delays on which standard Lyapunov arguments are applied to study the stability. Low-pass filtering capability of mollifiers is demonstrated for a high amplitude and rapidly oscillating noise. The controller is supported by numerical simulations.
- Synchronization:
  - In [12], we study a robust synchronization problem for multistable systems evolving on manifolds within an Input-to-State Stability (ISS) framework. Based on a recent generalization of the classical ISS theory to multistable systems, a robust synchronization protocol is designed with respect to a compact invariant set of the unperturbed system. The invariant set is assumed to admit a decomposition without cycles, that is, with neither homoclinic nor heteroclinic orbits. Numerical simulation examples illustrate our theoretical results.
  - In [51], [96], motivated by a recent work of R. Brockett Brockett (2013), we study a robust synchronization problem for multistable Brockett oscillators within an Input-to-State Stability (ISS) framework. Based on a recent generalization of the classical ISS theory to multistable systems and its application to the synchronization of multistable systems, a synchronization protocol is designed with respect to compact invariant sets of the unperturbed Brockett oscillator. The invariant sets are assumed to admit a decomposition without cycles (i.e. with neither homoclinic nor heteroclinic orbits). Contrarily to the local analysis of Brockett (2013), the conditions obtained in our work are global and applicable for family of non-identical oscillators. Numerical simulation examples illustrate our theoretical results.

7.5. Non-Linear, Sampled-Data And Time-Delay Systems

- Time-delay systems:
  - The problem of delay estimation for a class of nonlinear time-delay systems is considered in [82]. The theory of non-commutative rings is used to analyze the identifiability. Sliding mode technique is utilized in order to estimate the delay showing the possibility to have a local (or global) delay estimation for periodic (or aperiodic) delay signals.
  - In [14] we give sufficient conditions guaranteeing the observability of singular linear systems with commensurable delays affected by unknown inputs appearing in both the state equation and the output equation. These conditions allow for the reconstruction of the entire state vector using past and actual values of the system output. The obtained conditions coincide with known necessary and sufficient conditions of singular linear systems without delays.
  - [67] presents a finite-time observer for linear time-delay systems. In contrast to many observers, which normally estimate the system state in an asymptotic fashion, this observer estimates the exact system state in predetermined finite time. The finite-time observer proposed is achieved by updating the observer state based on actual and pass data of the observer. Simulation results are also presented to illustrate the convergence behavior of the finite-time observer.
  - The backward observability (BO) of a part of the vector of trajectories of the system state is tackled in [57] for a general class of linear time-delay descriptor systems with unknown inputs. By following a recursive algorithm, we present easy testable sufficient conditions ensuring the BO of descriptor time-delay systems.

  - Motivated by the problem of phase-locking in droop-controlled inverter-based microgrids with delays, in [23], the recently developed theory of input-to-state stability (ISS) for multistable systems is extended to the case of multistable systems with delayed dynamics. Sufficient conditions for ISS of delayed systems are presented using Lyapunov-Razumikhin functions. It is shown that ISS multistable systems are robust with respect to delays in a feedback. The derived theory is applied to two examples. First, the ISS property is established for the model of a nonlinear pendulum and delay-dependent robustness conditions are derived. Second, it is shown that, under certain assumptions, the problem of phase-locking analysis in droop-controlled inverter-based microgrids with delays can be reduced to the stability investigation of the nonlinear pendulum. For this case, corresponding delay-dependent conditions for asymptotic phase-locking are given.
  - Causal and non-causal observability are discussed in [68] for nonlinear time- delay systems. By extending the Lie derivative for time-delay systems in the algebraic framework introduced by Xia et al. (2002), we present a canonical form and give sufficient condition in order to deal with causal and non-causal observations of state and unknown inputs of time-delay systems.
  - [83] presents a finite-time observer for linear time-delay systems with commensurate delay. Unlike the existing observers in the literature which converges asymptotically, the proposed observer provides a finite-time estimation. This is realized by using the well-known sliding mode technique. Simulation results are also presented in order to illustrate the feasibility of the proposed method.
- Sampled-Data systems:
  - [104] presents basic concepts and recent research directions about the stability of sampled-data systems with aperiodic sampling. We focus mainly on the stability problem for systems with arbitrary time-varying sampling intervals which has been addressed in several areas of research in Control Theory. Systems with aperiodic sampling can be seen as time-delay systems, hybrid systems, Input/Output interconnections, discrete-time systems with time-varying parameters, etc. The goal of the article is to provide a structural overview of the progress made on the stability analysis problem. Without being exhaustive, which would be neither possible nor useful, we try to bring together results from diverse communities and present them in a unified manner. For each of the existing approaches, the basic concepts, fundamental results, converse stability theorems (when available), and relations with the other approaches are discussed in detail. Results concerning extensions of Lyapunov and frequency domain methods for systems with aperiodic sampling are recalled, as they allow to derive constructive stability conditions. Furthermore, numerical criteria are presented while indicating the sources of conservatism, the problems that remain open and the possible directions of improvement. At last, some emerging research directions, such as the design of stabilizing sampling sequences, are briefly discussed.
  - In [31] we investigate the stability analysis of nonlinear sampled-data systems, which are affine in the input. We assume that a stabilizing controller is designed using the emulation technique. We intend to provide sufficient stability conditions for the resulting sampled-data system. This allows to find an estimate of the upper bound on the asynchronous sampling intervals, for which stability is ensured. The main idea of the paper is to address the stability problem in a new framework inspired by the dissipativity theory. Furthermore, the result is shown to be constructive. Numerically tractable criteria are derived using linear matrix inequality for polytopic systems and using sum of squares technique for the class of polynomial systems.
  - [76] deals with the sampled-data control problem based on state estimation for linear sampled-data systems. An impulsive system approach is proposed based on a vector Lyapunov function method. Observer-based control design conditions are expressed in terms of LMIs. Some examples illustrate the feasibility of the proposed approach.

7.6. Effective algebraic systems theory

- Algebraic analysis approach:
  - The purpose of [97] is to present a survey on the effective algebraic analysis approach to linear systems theory with applications to control theory and mathematical physics. In particular, we show how the combination of effective methods of computer algebra – based on Gröbner basis techniques over a class of noncommutative polynomial rings of functional operators called Ore algebras – and constructive aspects of module theory and homological algebra enables the characterization of structural properties of linear functional systems. Algorithms are given and a dedicated implementation, called OREALGEBRAICANALYSIS, based on the Mathematica package HOLONOMICFUNCTIONS, is demonstrated.
  - As far as we know, there is no algebraic (polynomial) approach for the study of linear differential time-delay systems in the case of a (sufficiently regular) time-varying delay. Based on the concept of skew polynomial rings developed by Ore in the 30s, the purpose of [73] is to construct the ring of differential time-delay operators as an Ore extension and to analyze its properties. Classical algebraic properties of this ring, such as noetherianity, its homological and Krull dimensions and the existence of Gröbner bases, are characterized in terms of the time-varying delay function. In conclusion, the algebraic analysis approach to linear systems theory allows us to study linear differential time-varying delay systems (e.g. existence of autonomous elements, controllability, parametrizability, flatness, behavioral approach) through methods coming from module theory, homological algebra and constructive algebra.
  - Within the algebraic analysis approach to linear systems theory, in [98], we investigate the equivalence problem of linear functional systems, i.e., the problem of characterizing when all the solutions of two linear functional systems are in a one-to-one correspondence. To do that, we first provide a new characterization of isomorphic finitely presented modules in terms of inflations of their presentation matrices. We then prove several isomorphisms which are consequences of the unimodular completion problem. We then use these isomorphisms to complete and refine existing results concerning Serre's reduction problem. Finally, different consequences of these results are given. All the results obtained are algorithmic for rings for which Gröbner basis techniques exist and the computations can be performed by the Maple packages OREMODULES and OREMORPHISMS.
  - In [99], we study algorithmic aspects of the algebra of linear ordinary integro-differential operators with polynomial coefficients. Even though this algebra is not Noetherian and has zero divisors, Bavula recently proved that it is coherent, which allows one to develop an algebraic systems theory over this algebra. For an algorithmic approach to linear systems of integro-differential equations with boundary conditions, computing the kernel of matrices with entries in this algebra is a fundamental task. As a first step, we have to find annihilators of integro-differential operators, which, in turn, is related to the computation of polynomial solutions of such operators. For a class of linear operators including integro-differential operators, we present an algorithmic approach for computing polynomial solutions and the index. A generating set for right annihilators can be constructed in terms of such polynomial solutions. For initial value problems, an involution of the algebra of integro-differential operators then allows us to compute left annihilators, which can be interpreted as compatibility conditions of integro-differential equations with boundary conditions.
  - Recent progress in computer algebra has opened new opportunities for the parameter estimation problem in nonlinear control theory, by means of integro-differential input-output equations. In [102], we recall the origin of integro-differential equations. We present new opportunities in nonlinear control theory. Finally, we review related recent theoretical approaches on integro-differential algebras, illustrating what an integro-differential elimination method might be and what benefits the parameter estimation problem would gain from

it.

- Computational real algebraic geometric approach:
  - In [74], we present a symbolic-numeric method for solving the H_∞ loop-shaping design problem for low order single-input single-output systems with parameters. Due to the system parameters, no purely numerical algorithm can indeed solve the problem. Using Gröbner basis techniques and the Rational Univariate Representation of zero-dimensional algebraic varieties, we first give a parametrization of all the solutions of the two Algebraic Riccati Equations associated with the H_∞ control problem. Then, following some works on the spectral factorization problem, a certified symbolic-numeric algorithm is obtained for the computation of the positive definite solutions of these two Algebraic Riccati Equations. Finally, we present a certified symbolic-numeric algorithm which solves the H_∞ loop-shaping design problem for the above class of systems.
  - In [58], the asymptotic stability of linear differential systems with commensurate delays is studied. A classical approach for checking that all the roots of the corresponding quasipolynomial have negative real parts consists in computing the set of critical zeros of the quasipolynomial, i.e., the roots (and the corresponding delays) of the quasipolynomial that lie on the imaginary axis, and then analyzing the variation of these roots with respect to the variation of the delay. Based on solving algebraic systems techniques, a certified and efficient symbolic-numeric algorithm for computing the set of critical roots of a quasipolynomial is proposed. Moreover, using recent algorithmic results developed by the computer algebra community, we present an efficient algorithm for the computation of Puiseux series at a critical zero which allows us to finely analyze the stability of the system with respect to the variation of the delay.
  - In [59], we present new computer algebra based methods for testing the structural stability of n-D discrete linear systems (with $n \geq 2$). More precisely, we show that the standard characterization of the structural stability of a multivariate rational transfer function (namely, the denominator of the transfer function does not have solutions in the unit polydisc of $\mathbb{C}^n$) is equivalent to fact that a certain system of polynomials does not have real solutions. We then use state-of-the-art algorithms of the computer algebra community to check this last condition, and thus the structural stability of multidimensional systems.

7.7. Applications

- A fault detection method for an automatic detection of spawning in oysters [13]:

  Using measurements of valve activity (i.e. the distance between the two valves) in populations of bivalves under natural environmental condition (16 oysters in the Bay of Arcachon, France, in 2007, 2013 and 2014), an algorithm for an automatic detection of the spawning period of oysters is proposed in this paper. Spawning observations are important in aquaculture and biological studies, and until now, such a detection is done through visual analysis by an expert. The algorithm is based on the fault detection approach and it works through the estimation of velocity of valve movement activity, that can be obtained by calculating the time derivative of the valve distance. A summarized description of the methods used for the derivative estimation is provided, followed by the associated signal processing and decision making algorithm to determine spawning from the velocity signal. A protection from false spawning detection is also considered by analyzing the simultaneity in spawning. Through this study, it is shown that spawning in a population of oysters living in their natural habitat (i.e. in the sea) can be automatically detected without any human expertise saving time and resources. The fault detection method presented in the paper can also be used to detect complex oscillatory behavior which is of interest to control engineering community.

- Robust synchronization of genetic oscillators [52]:

Cell division introduces discontinuities in the dynamics of genetic oscillators (circadian clocks, synthetic oscillators, etc.) causing phase drift. This paper considers the problem of phase synchronization for a population of genetic oscillators that undergoes cell division and with a common entraining input in the population. Inspired by stochastic simulation, this paper proposes analytical conditions that guarantee phase synchronization. This analytical conditions are derived based on Phase Response Curve (PRC) model of an oscillator (the first order reduced model obtained for the linearized system and inputs with sufficiently small amplitude). Cell division introduces state resetting in the model (or phase resetting in the case of phase model), placing it in the class of hybrid systems. It is shown through numerical experiments for a motivating example that without common entraining input in all oscillators, the cell division acts as a disturbance causing phase drift, while the presence of entrainment guarantees boundedness of synchronization phase errors in the population. Theoretical developments proposed in the paper are demonstrated through numerical simulations for two different genetic oscillator models (Goodwin oscillator and Van der Pol oscillator).

- Modeling pointing tasks in mouse-based human-computer interactions [54]:

  Pointing is a basic gesture performed by any user during human-computer interaction. It consists in covering a distance to select a target via the cursor in a graphical user interface (e.g. a computer mouse movement to select a menu element). In this work, a dynamic model is proposed to describe the cursor motion during the pointing task. The model design is based on experimental data for pointing with a mouse. The obtained model has switched dynamics, which corresponds well to the state of the art accepted in the human-computer interaction community. The conditions of the model stability are established. The presented model can be further used for the improvement of user performance during pointing tasks.

- Modeling and control of turbulent flows [64]:

  The model-based closed-loop control of a separated flow can be studied based on the model described by Navier-Stokes equation. However, such a model still rises difficult issues for control practice. An alternative bilinear and delayed model has been developed tested on the experiments allowing its identification. The identification technique combines least-square technique with a Mesh Adaptive Direct Search (MADS) algorithm.

- Practical design considerations for successful industrial application of model-based fault detection techniques to aircraft systems [47]:

  This paper discusses some key factors which may arise for successful application of model-based Fault Detection(FD) techniques to aircraft systems. The paper reports on the results and the lessons learned during flight V & V(Validation & Verification) activities, implementation in the A380 Flight Control Computer(FCC) and A380 flight tests at Airbus(Toulouse, France).The paper does not focus on new theoretical materials, but rather on a number of practical design considerations to provide viable technological solutions and mechanization schemes. The selected case studies are taken from past and on-going research actions between Airbus and the University of Bordeaux (France). One of the presented solutions has received final certification on new generation Airbus A350 aircraft and is flying (first commercial flight: January 15,2015)

- Finite-time obstacle avoidance for unicycle-like robot [26]:

  The problem of avoiding obstacles while navigating within an environment for a Unicycle-like Wheeled Mobile Robot (WMR) is of prime importance in robotics; the aim of this work is to solve such a problem proposing a perturbed version of the standard kinematic model able to compensate for the neglected dynamics of the robot. The disturbances are considered additive on the inputs and the solution is based on the supervisory control framework, finite-time stability and a robust multi-output regulation. The effectiveness of the solution is proved, supported by experiments and finally compared with the Dynamic Window Approach (DWA) to show how the proposed method can perform better than standard methods.

- Almost global attractivity of a synchronous generator connected to an infinite bus [56]:

The problem of deriving verifiable conditions for stability of the equilibria of a realistic model of a synchronous generator with constant field current connected to an infinite bus is studied in the paper. Necessary and sufficient conditions for existence and uniqueness of equilibrium points are provided. Furthermore, sufficient conditions for almost global attractivity are given. To carry out this analysis a new Lyapunov–like function is proposed to establish convergence of bounded trajectories, while the latter is proven using the powerful theoretical framework of cell structures pioneered by Leonov and Noldus.

QUANTIC Project-Team

6. New Results

6.1. Observing Quantum State Diffusion by Heterodyne Detection of Fluorescence

Participants: Benjamin Huard, Mazyar Mirrahimi, Pierre Rouchon, Alain Sarlette, Pierre Six.

The results of this section were published in [16] and in [17].

Light emitted via fluorescence is associated with matter decaying in energy, and this light can be viewed as a probe that carries information about the state of its emitter. When this information is lost, the fragile quantum properties of the emitter are destroyed, a process known as decoherence. Using a superconducting qubit, we demonstrate how the sole measurement of fluorescence makes it possible to accurately track the quantum state in time. The observed evolution is erratic, which is expected based on the random backaction of measurements in quantum mechanics.

We continuously measure the amplitude of the fluorescence field emitted by a superconducting qubit using an amplifier close to the quantum limit; our measurements are obtained at cryogenic temperatures. From each fluorescence record, we can reconstruct a quantum trajectory, which is the succession of states the qubit occupies on a single relaxation event. We collect independent measurements of the qubit state at an arbitrary time during relaxation. These measurements follow the statistics that are expected from the quantum trajectories, thereby verifying the reconstructed quantum states. By repeating the experiment millions of times, we are able to determine the distribution of quantum trajectories. Strikingly, monitoring fluorescence can generate a superposition of states and counterintuitively lead to a temporary increase in the qubit excitation probability.

Our work provides an experimental demonstration of the quantum-state diffusion associated with spontaneous emission that triggered the field of quantum trajectories in the 1990s. We expect that our findings, which enlighten the correspondence between decoherence and measurement by the environment, will contribute to the progress of quantum error correction.

In a parallel work, we theoretically investigate statistical properties of the diffusion. In particular, we use a path integral formulation to determine the most likely trajectory during an evolution.

This work was made in collaboration with the team of Andrew Jordan at University of Rochester.

6.2. Using Spontaneous Emission of a Qubit as a Resource for Feedback Control

Participants: Nathanael Cottet, Benjamin Huard, Sebastien Jezouin, François Mallet, Pierre Rouchon, Alain Sarlette, Pierre Six.

The results of this section were published in [15].

We performed an experiment that demonstrates the permanent stabilization of any state of a superconducting qubit despite decoherence using a feedback scheme based on the information leaking out by the relaxation channel itself when the qubit spontaneously emits a photon.

At first sight, it may seem that using the detection of the photon that a qubit emits during a relaxation event cannot allow to protect an arbitrary quantum state from decoherence. First, it is very hard to collect efficiently the photons emitted by a two-level system. Second, the information contained in the emitted photon alone does not seem to be sufficient to correct the effect of relaxation and stabilize an arbitrary qubit state.

However, as we recently showed experimentally (see previous paragraph), it is now possible to measure the spontaneously emitted field using heterodyne detection, and reconstruct the quantum trajectory of a qubit. The information is therefore indeed useful and accessible!

Here, we go well beyond this previous work by not only decoding but also using the information contained in the spontaneously emitted field in real time. Specifically, we use the information contained in fluorescence to stabilize permanently any chosen state of the qubit by measurement feedback.

Stabilizing qubits by a feedback protocol based on the measurement of their relaxation channel had been proposed about 20 years ago by Hofmann and coworkers. They had claimed that it is possible to stabilize any state in the Southern hemisphere of the Bloch sphere. Wang and Wiseman revisited this problem 15 years ago and proposed a scheme that stabilizes any state of the Bloch sphere except the equator. In our work, we devise a new scheme that stabilizes any state, even on the equator! We are also the first ones to implement any such scheme experimentally.

The experiment itself covers several premieres, which are of wider interest to the quantum information and quantum control communities. First, we reach an unprecedented 35% of measurement efficiency for the spontaneously emitted photons out of a qubit (crucial parameter for feedback control). Second, this is the first multiple-input multiple-output feedback in the quantum regime. Finally, we devise a new feedback controller based on the ac-Stark effect to tune the qubit frequency as a function of one input analog signal.

6.3. Well-posedness and convergence of the Lindblad master equation for a quantum harmonic oscillator with multi-photon drive and damping

Participants: Remi Azouit, Pierre Rouchon, Alain Sarlette

The main motivation for this result was to finally treat in a rigorous way the convergence of a non-trivial infinite-dimensional system (harmonic oscillator Hilbert space) that is of relevance to physicists. The essential tools for this proof are the choice of an appropriate metric leading to contraction, and the Hille-Yosida theorem ensuring well-posedness of the problem. This could be a valuable basis towards a more general, yet easily invocable argument to treat the many other infinite-dimensional quantum dynamics which intuitively "should never escape towards infinite energies."

This result has been published in [13].

6.4. Quantum state tomography with non-instantaneous measurements, imperfections, and decoherence

Participants: Pierre Six, Alain Sarlette, Benjamin Huard, Pierre Rouchon

Tomography of a quantum state is usually based on positive operator-valued measure (POVM) and on their experimental statistics. Among the available reconstructions, the maximum-likelihood (MaxLike) technique is an efficient one. We propose an extension of this technique when the measurement process cannot be simply described by an instantaneous POVM. Instead, the tomography relies on a set of quantum trajectories and their measurement records. This model includes the fact that, in practice, each measurement could be corrupted by imperfections and decoherence, and could also be associated with the record of continuous-time signals over a finite amount of time. The goal is then to retrieve the quantum state that was present at the start of this measurement process. The proposed extension relies on an explicit expression of the likelihood function via the effective matrices appearing in quantum smoothing and solutions of the adjoint quantum filter. It allows to retrieve the initial quantum state as in standard MaxLike tomography, but where the traditional POVM operators are replaced by more general ones that depend on the measurement record of each trajectory. It also provides, aside the MaxLike estimate of the quantum state, confidence intervals for any observable. Such confidence intervals are derived, as the MaxLike estimate, from an asymptotic expansion of multi-dimensional Laplace integrals appearing in Bayesian Mean estimation. This work should allow much more accurate inference of the state achieved by some quantum experiment, before a non-instantaneous measurement process is performed to check its results – distinguishing the loss in fidelity truly incurred by the preparation process, from the loss in fidelity induced only by the benchmarking measurement process which would not be present in the final application. A validation is performed on two sets of experimental data: photon(s) trapped in a microwave cavity subject to quantum non-demolition measurements relying on Rydberg atoms, where we have collaborated with the group of Igor Dotsenko at the LKB, College de France; and the heterodyne fluorescence measurements of a superconducting qubit, with the experimentalists of the QUANTIC team.

This result has been published in [27].

6.5. Adiabatic elimination for open quantum systems with effective Lindblad master equations

Participants: Remi Azouit, Pierre Rouchon, Alain Sarlette

We consider an open quantum system described by a Lindblad-type master equation with two times-scales. The fast time-scale is strongly dissipative and drives the system towards a low-dimensional decoherence-free space. To perform the adiabatic elimination of this fast relaxation, we propose a geometric asymptotic expansion based on the small positive parameter describing the time-scale separation. This expansion exploits geometric singular perturbation theory and center-manifold techniques. We conjecture that, at any order, it provides an effective slow Lindblad master equation and a completely positive parameterization of the slow invariant sub-manifold associated to the low-dimensional decoherence-free space. By preserving complete positivity and trace, two important structural properties attached to open quantum dynamics, we obtain a reduced-order model that directly conveys a physical interpretation since it relies on effective Lindbladian descriptions of the slow evolution. At the first order, we derive simple formulae for the effective Lindblad master equation. For a specific type of fast dissipation, we show how any Hamiltonian perturbation yields Lindbladian second-order corrections to the first-order slow evolution governed by the Zeno-Hamiltonian. These results are illustrated on a composite system made of a strongly dissipative harmonic oscillator, the ancilla, weakly coupled to another quantum system.

This result has been published in [30].

6.6. Loss-tolerant parity measurement for distant quantum bits

Participants: Mazyar Mirrahimi, Alain Sarlette

We propose a scheme to measure the parity of two distant qubits, while ensuring that losses on the quantum channel between them does not destroy coherences within the parity subspaces. This last property is a new and essential feature towards using repeated parity measurements in realistic physical conditions. It is achieved thanks to the use of cat states for the probe field that interacts with the two remote qubits. We show how this allows to stabilize highly entangled states between distant qubits, with the current state-of-the-art circuit QED capabilities. Highly entangled states are envisioned as a fundamental building block of the so-called modular quantum computing architecture, so their stabilization, i.e rapid availability, can be viewed as a major step towards enabling such technology.

This result has been submitted as a journal paper [23].

6.7. Holonomic quantum control with continuous variable systems

Participants: Mazyar Mirrahimi

In a collaboration with the team of Liang Jiang at Yale University we propose a scheme to realize a set of universal gates on protected cat-qubits. Universal computation of a quantum system consisting of superpositions of well-separated coherent states of multiple harmonic oscillators can be achieved by three families of adiabatic holonomic gates. The first gate consists of moving a coherent state around a closed path in phase space, resulting in a relative Berry phase between that state and the other states. The second gate consists of “colliding” two coherent states of the same oscillator, resulting in coherent population transfer between them. The third gate is an effective controlled-phase gate on coherent states of two different oscillators. Such gates should be realizable via reservoir engineering of systems that support tunable nonlinearities, such as trapped ions and circuit QED.

This result has been published in [11].

6.8. A Schrodinger cat living in two boxes

Participants: Mazyar Mirrahimi

Quantum superpositions of distinct coherent states in a single-mode harmonic oscillator, known as cat states, have been an elegant demonstration of Schrodinger's famous cat paradox. Here, in a collaboration with the team of Robert Schoelkopf at Yale university, we realize a two-mode cat state of electromagnetic fields in two microwave cavities bridged by a superconducting artificial atom, which can also be viewed as an entangled pair of single-cavity cat states. We present full quantum state tomography of this complex cat state over a Hilbert space exceeding 100 dimensions via quantum nondemolition measurements of the joint photon number parity. The ability to manipulate such multicavity quantum states paves the way for logical operations between redundantly encoded qubits for fault-tolerant quantum computation and communication.

This result has been published in [28].

6.9. Extending the lifetime of a quantum bit with error correction in superconducting circuits

Participants: Zaki Leghtas, Mazyar Mirrahimi

Quantum error correction (QEC) can overcome the errors experienced by qubits and is therefore an essential component of a future quantum computer. To implement QEC, a qubit is redundantly encoded in a higher-dimensional space using quantum states with carefully tailored symmetry properties. Projective measurements of these parity-type observables provide error syndrome information, with which errors can be corrected via simple operations. The break-even point of QEC at which the lifetime of a qubit exceeds the lifetime of the constituents of the system has so far remained out of reach. Although previous works have demonstrated elements of QEC, they primarily illustrate the signatures or scaling properties of QEC codes rather than test the capacity of the system to preserve a qubit over time. Here, in a collaboration with the team of Robert Schoelkopf at Yale University, we demonstrate a QEC system that reaches the break-even point by suppressing the natural errors due to energy loss for a qubit logically encoded in superpositions of Schrodinger-cat states of a superconducting resonator. We implement a full QEC protocol by using real-time feedback to encode, monitor naturally occurring errors, decode and correct. As measured by full process tomography, without any post-selection, the corrected qubit lifetime is 320 microseconds, which is longer than the lifetime of any of the parts of the system: 20 times longer than the lifetime of the transmon, about 2.2 times longer than the lifetime of an uncorrected logical encoding and about 1.1 longer than the lifetime of the best physical qubit (Fock states of the resonator). Our results illustrate the benefit of using hardware-efficient qubit encodings rather than traditional QEC schemes. Furthermore, they advance the field of experimental error correction from confirming basic concepts to exploring the metrics that drive system performance and the challenges in realizing a fault-tolerant system.

This result has been published in [22].

6.10. Robust Concurrent Remote Entanglement Between Two Superconducting Qubits

Participants: Zaki Leghtas

Entangling two remote quantum systems that never interact directly is an essential primitive in quantum information science and forms the basis for the modular architecture of quantum computing. When protocols to generate these remote entangled pairs rely on using traveling single-photon states as carriers of quantum information, they can be made robust to photon losses, unlike schemes that rely on continuous variable states. However, efficiently detecting single photons is challenging in the domain of superconducting quantum circuits because of the low energy of microwave quanta. Here, in a collaboration with the team of Michel

Devoret at Yale University, we report the realization of a robust form of concurrent remote entanglement based on a novel microwave photon detector implemented in the superconducting circuit quantum electrodynamics platform of quantum information. Remote entangled pairs with a fidelity of 0.57 are generated at 200 Hz. Our experiment opens the way for the implementation of the modular architecture of quantum computation with superconducting qubits.

This work was published in [21].

6.11. Planar Multilayer Circuit Quantum Electrodynamics

Participants: Zaki Leghtas

Experimental quantum information processing with superconducting circuits is rapidly advancing, driven by innovation in two classes of devices, one involving planar microfabricated (2D) resonators, and the other involving machined three-dimensional (3D) cavities. In a collaboration with the team of Michel Devoret at Yale University, we demonstrate that circuit quantum electrodynamics can be implemented in a multilayer superconducting structure that combines 2D and 3D advantages. We employ standard microfabrication techniques to pattern each layer, and rely on a vacuum gap between the layers to store the electromagnetic energy. Planar qubits are lithographically defined as an aperture in a conducting boundary of the resonators. We demonstrate the aperture concept by implementing an integrated, two-cavity-mode, one-transmon-qubit system.

This work was published in [19].

6.12. Theory of remote entanglement via quantum-limited phase-preserving amplification

Participants: Zaki Leghtas

In a collaboration with the teams of Steven Girvin and Michel Devoret at Yale University, we show that a quantum-limited phase-preserving amplifier can act as a which-path information eraser when followed by heterodyne detection. This “beam splitter with gain” implements a continuous joint measurement on the signal sources. As an application, we propose heralded concurrent remote entanglement generation between two qubits coupled dispersively to separate cavities. Dissimilar qubit-cavity pairs can be made indistinguishable by simple engineering of the cavity driving fields providing further experimental flexibility and the prospect for scalability. Additionally, we find an analytic solution for the stochastic master equation, a quantum filter, yielding a thorough physical understanding of the nonlinear measurement process leading to an entangled state of the qubits. We determine the concurrence of the entangled states and analyze its dependence on losses and measurement inefficiencies.

This work was published in [26].

SPHINX Project-Team

7. New Results

7.1. Analysis, control and stabilization of heterogeneous systems

Participant: Takéo Takahashi.

In [12], T. Takahashi (with D. Maity and M. Tucsnak, both from Institut de Mathématiques de Bordeaux, France) has considered a free boundary problem modeling the motion of a piston in a viscous gas. The gas-piston system fills a cylinder with fixed extremities, which possibly allow gas from the exterior to penetrate inside the cylinder. The gas is modeled by the 1D compressible Navier-Stokes system and the piston motion is described by the second Newton law. They prove the existence and uniqueness of global in time strong solutions. The main novelty brought in is that the case of nonhomogeneous boundary conditions is considered. Moreover, even for homogeneous boundary conditions, their results require less regularity of the initial data than those obtained in previous works.

In [32], T. Takahashi (with C. Lacave from Institut Fourier, Grenoble, France) has studied the motion of a single disk moving under the influence of a 2D viscous fluid. They deal with the asymptotic as the size of the solid tends to zero. If the density of the solid is independent of the size of the solid, the energy equality is not sufficient to obtain a uniform estimate for the solid velocity. This will be achieved thanks to the optimal $L^p - L^q$ decay estimates of the semigroup associated to the fluid-rigid body system and to a fixed point argument. Next, they deduce the convergence to the solution of the Navier-Stokes equations in $\mathbb{R}^2$.

In [7], T. Takahashi (with C. Bianchini (Dimai, Florence, Italy) and A. Henrot (IECL, Nancy, France)) has tackled a model for the shape of vesicles. In order to do this, they consider a shape optimization problem associated with a Willmore type energy in the plane. More precisely, they study a *Blaschke-Santaló diagram* involving the area, the perimeter and the elastic energy of planar convex bodies. Existence, regularity and geometric properties of solutions to this shape optimization problem are shown.

We have studied the self-propelled motions of a rigid body immersed in a viscous incompressible fluid which fills the exterior domain of the rigid body. The mechanism used by the body to reach the desired motion is modeled through a distribution of velocities at its boundary.

T. Takahashi (with J. San Martín (DIM, Santiago, Chile) and M. Tucsnak (Institut de Mathématiques de Bordeaux, France)) considers in [16] a class of swimmers of low Reynolds number, of prolate spheroidal shape, which can be seen as simplified models of ciliated microorganisms. Within this model, the form of the swimmer does not change, the propelling mechanism consisting in tangential displacements of the material points of swimmer's boundary. Using explicit formulas for the solution of the Stokes equations at the exterior of a translating prolate spheroid the governing equations reduce to a system of ODE's with the control acting in some of its coefficients (bilinear control system). The main theoretical result asserts the exact controllability of the prolate spheroidal swimmer. In the same geometrical situation, they define a concept of efficiency which reduces to the classical one in the case of a spherical swimmer and they consider the optimal control problem of maximizing this efficiency during a stroke. Moreover, they analyse the sensitivity of this efficiency with respect to the eccentricity of the considered spheroid. They provide semi-explicit formulas for the Stokes equations at the exterior of a prolate spheroid, with an arbitrary tangential velocity imposed on the fluid-solid interface. Finally, they use numerical optimization tools to investigate the dependence of the efficiency on the number of inputs and on the eccentricity of the spheroid. The "best" numerical result obtained yields an efficiency of 30.66% with 13 scalar inputs. In the limiting case of a sphere their best numerically obtained efficiency is of 30.4%, whereas the best computed efficiency previously reported in the literature was of 22%.

In [10], T. Takahashi (with T. Hishida (Nagoya University, Japan) and A.L. Silvestre (IST, Lisboa, Portugal)) tackles the stationary case. The fluid motion is modeled by the stationary Navier-Stokes system coupled with two relations for the balance of forces and torques. They prove that there exists a control allowing the rigid body to move with a prescribed rigid velocity provided the velocity is small enough. They also show that since the net force exerted by the fluid to the rigid body vanishes, we have a better summability of the fluid velocity than the classical summability result for the solutions of the stationary Navier-Stokes system in exterior domains.

7.2. Inverse problems for heterogeneous systems

Participants: David Dos Santos Ferreira, Alexandre Munnier, Karim Ramdani, Julie Valein, Jean-Claude Vivalda.

Many inverse problems (IP) appearing in fluid-structure interaction and wave propagation problems have been investigated in the team.

In [14], Munnier and Ramdani consider the 2D inverse problem of recovering the positions and the velocities of slowly moving small rigid disks in a bounded cavity filled with a perfect fluid. Using an integral formulation, they first derive an asymptotic expansion of the DtN map of the problem as the diameters of the disks tend to zero. Then, combining a suitable choice of exponential type data and the DORT method (French acronym for Diagonalization of the Time Reversal Operator), a reconstruction method for the unknown positions and velocities is proposed. Let us emphasize here that this reconstruction method uses in the context of fluid-structure interaction problems a method which is usually used for waves inverse scattering (the DORT method).

In [13], Munnier and Ramdani propose a new method to tackle a geometric inverse problem related to Calderón's inverse problem. More precisely, they propose an explicit reconstruction formula for the cavity inverse problem using conformal mapping. This formula is derived by combining two ingredients: a new factorization result of the DtN map and the so-called generalized Pólia-Szegö tensors of the cavity.

In [9], P. Caro (Department of Mathematics and Statistics, Helsinki, Finland), D. Dos Santos Ferreira and Alberto Ruiz (Instituto de Ciencias Matematicas, Madrid, Spain) obtained stability estimates for potentials in a Schrödinger equation in dimension higher than 3 from the associated Dirichlet-to-Neumann map with partial data. The estimates are of log-log type and represent a quantitative version of the uniqueness result of Kenig, Sjöstrand and Uhlmann. The proof is based on a reduction to a stability estimate on the attenuated geodesic ray transform on the hypersphere.

In [15], Ramdani, Tucsnak (Institut de Mathématiques de Bordeaux, France) and Valein tackle a state estimation problem for a system of infinite dimension arising in population dynamics (a linear model for age-structured populations with spatial diffusion). Assume the initial state to be unknown, the considered inverse problem is to estimate asymptotically on time the state of the system from a locally distributed observation in both age and space. This is done by designing a Luenberger observer for the system, taking advantage of the particular spectral structure of the problem (the system has a finite number of unstable eigenvalues).

In [2], Ammar (Faculté des Sciences de Sfax, Tunisia), Massaoud (Faculté des Sciences de Sfax, Tunisia) and Vivalda characterize the globally Lipschitz continuous systems defined on $\mathbb{R}^n$ whose observability is preserved under time sampling.

7.3. Numerical analysis and simulation of heterogeneous systems

Participants: Xavier Antoine, Mohamed El Bouajaji, Karim Ramdani, Qinglin Tang, Julie Valein, Chi-Ting Wu.

In optics, metamaterials (also known as negative or left-handed materials), have known a growing interest in the last two decades. These artificial composite materials exhibit the property of having negative dielectric permittivity and magnetic permeability in a certain range of frequency, leading hence to materials with negative refractive index and super lens effects. In [8], Bunoiu (IECL, Metz, France) and Ramdani consider a complex wave system involving such materials. More precisely, they consider a periodic homogenization problem involving two isotropic materials with conductivities of different signs: a classical material and a metamaterial (or negative material). Combining the $\mathbf{T}-$coercivity approach and the unfolding method for homogenization, they prove well-posedness results for the initial and the homogenized problems and obtain a convergence result, provided that the contrast between the two conductivities is large enough (in modulus).

In [18], Tucsnak (Institut de Mathématiques de Bordeaux, France), Valein and Wu study the numerical approximation of the solutions of a class of abstract parabolic time-optimal control problems with unbounded control operator. Our main results assert that, provided that the target is a closed ball centered at the origin and of positive radius, the optimal time and the optimal controls of the approximate time optimal problems converge (in appropriate norms) to the optimal time and to the optimal controls of the original problem. In order to prove our main theorem, we provide a nonsmooth data error estimate for abstract parabolic systems.

In [4], Antoine and Lorin (School of Mathematics and Statistics, Ottawa, and CRM, Montréal, Canada) analyze the convergence of optimized Schwarz domain decomposition methods for the simulation of the time-domain Schrödinger equation with high-order local transmission conditions.

In [5], Antoine, Tang and Zhang (WPI, Austria and IRMAR, France) develop some spectral methods for computing the ground states and dynamics of space fractional Gross-Pitaevskii equations arising in the modeling of fractional Bose-Einstein equations with long-range nonlinear interactions. In addition, we also state some existence and uniqueness properties for the ground states of such equations, and prove some dynamical laws.

In [6], Bao (Department of Mathematics, Singapore), Tang and Zhang (WPI, Austria and IRMAR, France) develop a new efficient and spectrally accurate numerical for computing the ground state and dynamics of dipolar Bose-Einstein condensates. They pay a particular attention to the computation of the nonlinear nonlocal interactions through the use of the nonuniform fast Fourier transform.

In [22], Antoine, Levitt (CERMICS, France) and Tang derive a highly accurate and efficient new numerical method for computing the ground states of the fast rotating Gross-Pitaevskii equation. The method is based on a preconditioned nonlinear conjugate gradient method which leads to a high gain compared to most recent approaches.

In [26], Bao (Department of Mathematics, Singapore), Cai (Department of mathematics Purdue University, USA and CSRC, Beijing, China), Jia (Department of Mathematics, Singapore), Tang develop a uniformly accurate multiscale time integrator in conjunction with a spectral method for computing the dynamics of the nonrelativistic Dirac equation. The same authors develop and compare, in [27], some new numerical methods for the simulation of the Dirac equation when the nonrelativistic regime is considered.

The article [17] is devoted to explain how the open finite element solver GetDDM works. The mathematical methods behind GetDDM are optimized Schwarz domain decomposition methods with well-designed transmission boundary conditions. GetDDM allows to solve large scale high frequency wave problems (e.g. acoustics, electromagnetism, elasticity problems) on large clusters. This papers explains through examples and scripts how GetDDM must be used. GetDDM is a result of a long term collaboration between Xavier Antoine and Christophe Geuzaine (University of Liège).

TROPICAL Team

7. New Results

7.1. Optimal control and zero-sum games

7.1.1. Fixed points of order preserving homogeneous maps and zero-sum games

Participants: Marianne Akian, Stéphane Gaubert, Antoine Hochart.

The PhD work of Antoine Hochart [12] deals with the applications of methods of non-linear fixed point theory to zero-sum games.

A highlight of his PhD is the characterization of the property of ergodicity for zero-sum games. In the special "zero-player" case, i.e., for a Markov chain equipped with an additive functional (payment) of the trajectory, the ergodicity condition entails that the mean payoff is independent of the initial state, for any choice of the payment. In the case of finite Markov chains, ergodicity admits several characterizations, including a combinatorial one (the uniqueness of the final class). This carries over to the two player case: ergodicity is now characterized by the absence of certain pairs of conjugate invariant sets (dominions), and it can be checked using directed hypergraphs algorithms. This leads to an explicit combinatorial sufficient condition for the solvability of the "ergodic equation", which is the main tool in the numerical approach of the mean payoff problem. These results appeared in [59], [58], [60]. A more general approach was developed in [30], in which zero-sum games are now studied abstractly in terms of accretive operators. This allows one to show that the bias vector (the solution of the ergodic equation) is unique for a generic perturbation of the payments.

Another series of results of the thesis concern the finite action space, showing that the set of payments for which the bias vector is not unique coincides with the union of lower dimensional cells of a polyhedral complex, which an application to perturbation schemes in policy iteration [47].

A last result of the thesis is a representation theorem for "payment free" Shapley operators, showing that these are characterized by monotonicity and homogeneity axioms [48]. This extends to the two-player case known representation theorems for risk measures.

7.1.2. Probabilistic and max-plus approximation of Hamilton-Jacobi-Bellman equations

Participants: Marianne Akian, Eric Fodjo.

The PhD thesis of Eric Fodjo concerns stochastic control problems obtained in particular in the modelisation of portfolio selection with transaction costs. The dynamic programming method leads to a Hamilton-Jacobi-Bellman partial differential equation, on a space with a dimension at least equal to the number of risky assets. The curse of dimensionality does not allow one to solve numerically these equations for a large dimension (greater to 5). We propose to tackle these problems with numerical methods combining policy iterations, probabilistic discretisations, max-plus discretisations, in order to increase the possible dimension. Another solution is to replace policy iterations by an approximation with optimal switching problems.

In [27], [26] (also presented in [35], [23]), we consider fully nonlinear Hamilton-Jacobi-Bellman equations associated to diffusion control problems with finite horizon involving a finite set-valued (or switching) control and possibly a continuum-valued control. We construct a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [93], [99] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [78] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. Numerical tests on a small example of pricing and hedging an option are presented. Moreover, more recently, we improved the method of Fahim, Touzi and Warin to allow one to solve fully nonlinear parabolic partial differential equations with general volatilities.

7.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

7.2.1. Isometries of the Hilbert geometry

Participant: Cormac Walsh.

In a collaboration with Bas Lemmens (Kent University, UK), we have been studying the Hilbert geometry in finite dimensions, especially its horofunction boundary and isometry group. The book chapter [117] contains a survey of this work. However, the infinite dimensional case is also interesting, and has been used as a tool for many years in non-linear analysis. Despite this, very little is known about the geometry of these spaces when the dimension is infinite.

An example of a problem in which we are interested is the following. In finite dimension it is known that a Hilbert geometry is isometric to a normed space if and only if it is a simplex. We have shown [118] that, more generally, a Hilbert geometry is isometric to a Banach space if and only if it is the cross-section of a positive cone, that is, the cone of positive continuous functions on some compact topological space. To solve this problem we found it useful to study the horofunction boundary in the infinite-dimensional case.

We are continuing to study similar problems in relation to this topic in collaboration with Bas Lemmens of the University of Kent.

7.2.2. Volume growth in the Hilbert geometry

Participant: Cormac Walsh.

In a collaboration with Constantin Vernicos of Université Montpellier 2, we are investigating how the volume of a ball in a Hilbert geometry grows as its radius increases. Specifically, we are studying the volume entropy

$$\lim_{r\to\infty} \frac{\log \mathrm{Vol}\, B(x,r)}{r}, \tag{8}$$

where $B(x,r)$ is the ball with center x and radius r, and Vol denotes some notion of volume, for example, the Holmes–Thompson or Busemann definitions. Note that the entropy does not depend on the particular choice of x, nor on the choice of the volume. It is known that the hyperbolic space, or indeed any Hilbert geometry with a C^2-smooth boundary of strictly positive curvature, has entropy $n-1$, where n is the dimension, and it has recently been proved that this is the maximal entropy possible for Hilbert geometries of the given dimension.

Constantin Vernicos has shown that, in dimension 2 and 3, the volume entropy of a Hilbert geometry on a convex body is equal to exactly twice the *approximability* of the body, that is, the power of $1/\epsilon$ governing the growth of the number of vertices needed to approximate the body by a polytope within ϵ, as ϵ decreases.

Studying polytopal Hilbert geometries, we have demonstrated [53] a close relation between the volume and the number of *flags* of the polytope, more precisely, that the volume of large balls is asymptotically proportional to the number of flags. This suggested to us defining a new notion of approximability using flags rather than vertices. We have shown [53] that the volume entropy of a Hilbert geometry on a convex body is equal to exactly twice this *flag-approximability* in all dimensions. This implies in particular that the volume entropy of a convex body is equal to that of its dual.

7.2.3. The set of minimal upper bounds of two matrices in the Loewner order

Participant: Nikolas Stott.

A classical theorem of Kadison shows that the space of symmetric matrices equipped with the Loewner order is an anti-lattice, meaning that two matrices have a least upper bound if and only if they are comparable. In [52], we refined this theorem by characterizing the set of minimal upper bounds: we showed that it is homeomorphic to the quotient space $O(p) \setminus O(p,q)/O(q)$, where $O(p,q)$ denotes the orthogonal group associated to the quadratic form with signature (p,q), and $O(p)$ denotes the standard pth orthogonal group.

7.2.4. Checking the strict positivity of Kraus maps is NP-hard

Participant: Stéphane Gaubert.

In collaboration with Zheng Qu (now with HKU, Hong Kong), I studied several decision problems arising from the spectral theory of Kraus maps (trace preserving completely positive maps), acting on the cone of positive semidefinite matrices. The latter appear in quantum information. We showed that checking the irreducibility (absence of non-trivial invariant face of the cone) and primitivity properties (requiring the iterates of the map to send the cone to its interior) can be checked in polynomial time, whereas checking positivity (whether the map sends the cone to its interior) is NP-hard. In [17], we studied complexity issues related to Kraus maps, and showed in particular that checking whether a Kraus map sends the cone to its interior is NP-hard.

7.3. Tropical algebra and convex geometry

7.3.1. Formalizing convex polyhedra in Coq

Participants: Xavier Allamigeon, Ricardo Katz [Conicet, Argentine].

We formalize a certain fragment of the theory of convex polyhedra and their combinatorial properties. Our motivation is that convex polyhedra are involved in a wide range of analysis techniques such as in formal verification, and that their combinatorial properties are used to establish more fundamental results, especially in tropical geometry.

This formalization has been conducted in Coq using the Mathematical Components library. We have implemented a full formalization of the simplex algorithm, which allows to make several key properties of convex polyhedra (feasibility, unboundedness, etc) decidable. From this, we have deduced a formal proof of strong duality theorem in linear programming, and of Farkas lemma. We also have a formal implementation of Motzkin's double description method, which provides a constructive way to prove Minkowski theorem for polyhedra.

7.3.2. Tropical totally positive matrices

Participants: Stéphane Gaubert, Adi Niv.

In [50], we investigate the tropical analogues of totally positive and totally non-negative matrices, i.e, the images by the valuation of the corresponding classes of matrices over a non-archimedean field. We show that tropical totally positive matrices essentially coincide with the Monge matrices (defined by the positivity of 2×2 tropical minors), arising in optimal transport. These results have been presented in [41], [40].

7.3.3. Tropical compound matrix identities

Participants: Marianne Akian, Stéphane Gaubert, Adi Niv.

In [55], [57], we proved some identities on matrices using a weak and a strong transfer principles. In the present work, we prove identities on compound matrices in extended tropical semirings. Such identities include analogues to properties of conjugate matrices, powers of matrices and $\mathrm{adj}\,(A)\det{(A)}^{-1}$, all of which have implications on the eigenvalues of the corresponding matrices. A tropical Sylvester-Franke identity is provided as well. Even though part of these identities hold over any commutative ring, they cannot be adjusted to semirings with symmetry using the existing weak and strong transfer principles. Here, we provide the proofs by means of graph theory arguments.

7.3.4. Supertropical algebra

Participant: Adi Niv.

Several properties of matrices over the tropical algebra are studied using the supertropical algebra introduced in [92].

The only invertible matrices in tropical algebra are diagonal matrices, permutation matrices and their products. However, the pseudo-inverse A^{∇}, defined as $\frac{1}{\det(A)}\,\mathrm{adj}\,(A)$, with $\det(A)$ being the tropical permanent, inherits some classical algebraic properties and has some surprising new ones. In [104], defining B and B' to be tropically similar if $B' = A^{\nabla}BA$, we examine the characteristic (max-)polynomials of tropically similar matrices as well as those of pseudo-inverses. Other miscellaneous results include a new proof of the identity for $\det(AB)$ and a connection to stabilization of the powers of definite matrices.

In a joint work with Louis Rowen (Bar Ilan Univ.) [21], we study the pathology that causes tropical eigenspaces of distinct supertropical eigenvalues of a non-singular matrix A, to be dependent. We show that in lower dimensions the eigenvectors of distinct eigenvalues are independent, as desired. The index set that differentiates between subsequent essential monomials of the characteristic polynomial, yields an eigenvalue λ, and corresponds to the columns of the eigenmatrix $A + \lambda I$ from which the eigenvectors are taken. We ascertain the cause for failure in higher dimensions, and prove that independence of the eigenvectors is recovered in case the “difference criterion” holds, defined in terms of disjoint differences between index sets of subsequent coefficients. We conclude by considering the eigenvectors of the matrix $A^{\nabla} := \frac{1}{\det(A)}\mathrm{adj}(A)$ and the connection of the independence question to generalized eigenvectors.

7.3.5. Volume and integer points of tropical polytopes

Participants: Marie Maccaig, Stéphane Gaubert.

We investigated the volume of tropical polytopes, as well as the number of integer points contained in integer polytopes. We proved that even approximating these values for a tropical polytope given by its vertices is hard, with no approximation algorithm with factor $2^{\mathrm{poly}(m,n)}$ existing. We further proved the $\sharp$P-hardness for the analogous problems for tropical polytopes instead defined by inequalities. We also investigated the relation between the set of integer points of a tropical polytope and the image by the valuation of polytopes over the nonarchimedean field of Puiseux series.

7.3.6. Primal dual pair of max-algebraic integer linear programs (MLP)

Participant: Marie Maccaig.

There are known weak and strong duality theorems for max-algebraic linear programs. I investigated the integer versions of these problems; considering the impact of requiring integer solutions instead of real solutions. I proved a tight bound on the duality gap for a pair of integer solutions to the primal and dual MLPs, and searched for conditions on when the optimal values of the integer primal and dual MLPs coincide.

7.3.7. Tropical Jacobi identity

Participants: Marie Maccaig, Adi Niv.

In a joint work with Sergei Sergeev (Birmingham), we investigated the combinatorial interpretation for the Tropical Jacobi identity. Inspired by Butkovic’s paper, "Max-algebra, the algebra of combinatorics?" and many other links between max-algebra and combinatorics, we try to link this tropical quantity to a new type of multiple assignment problem.

7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

7.4.1. Majorization inequalities for valuations of eigenvalues using tropical algebra

Participants: Marianne Akian, Stéphane Gaubert.

We consider a matrix with entries over the field of Puiseux series, equipped with its non-archimedean valuation (the leading exponent). In [13], with Ravindra Bapat (Univ. New Delhi), we establish majorization inequalities relating the sequence of the valuations of the eigenvalues of a matrix with the tropical eigenvalues of its valuation matrix (the latter is obtained by taking the valuation entrywise). We also show that, generically in the leading coefficients of the Puiseux series, the precise asymptotics of eigenvalues, eigenvectors and condition numbers can be determined. For this, we apply diagonal scalings constructed from the dual variables of a parametric optimal assignment constructed from the valuation matrix.

In recent works with Andrea Marchesini and Françoise Tisseur (Manchester University), we use the same technique to establish an archimedean analogue of the above inequalities, which applies to matrix polynomials with coefficients in the field of complex numbers, equipped with the modulus as its valuation. This allows us in particular to improve the accuracy of the numerical computation of the eigenvalues of such matrix polynomials.

In [15], with Meisam Sharify (IPM, Tehran, Iran), we also establish log-majorization inequalities of the eigenvalues of matrix polynomials using the tropical roots of some scalar polynomials depending only on the norms of the matrix coefficients. This extends to the case of matrix polynomials some bounds obtained by Hadamard, Ostrowski and Pólya for the roots of scalar polynomials.

These works have been presented in [22].

7.4.2. Tropicalization of the central path and application to the complexity of interior point methods

Participants: Xavier Allamigeon, Stéphane Gaubert.

This work is in collaboration with Pascal Benchimol (now with EDF Labs) and Michael Joswig (TU-Berlin).

In optimization, path-following interior point methods are driven to an optimal solution along a trajectory called the central path. The *central path* of a linear program LP$(A, b, c) \equiv \min\{c \cdot x \mid Ax \leq b, \ x \geq 0\}$ is defined as the set of the optimal solutions (x^μ, w^μ) of the barrier problems:

$$\begin{array}{ll} \text{minimize} & c \cdot x - \mu\left(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i\right) \\ \text{subject to} & Ax + w = b, \ \ x > 0, \ \ w > 0 \end{array}$$

While the complexity of interior point methods is known to be polynomial, an important question is to study the number of iterations which are performed by interior point methods, in particular whether it can be bounded by a polynomial in the dimension (mn) of the problem. This is motivated by one of Smale's problems, on the existence of a strongly polynomial complexity algorithm for linear programming. So far, this question has been essentially addressed though the study of the curvature of the central path, which measures how far a path differs from a straight line, see [75], [74], [77], [76]. In particular, by analogy with the classical Hirsch conjecture, Deza, Terlaky and Zinchencko [76] conjectured that $O(m)$ is also an upper bound for the total curvature.

In a work of X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig, we study the tropicalization of the central path. The *tropical central path* is defined as the logarithmic limit of the central paths of a parametric family of linear programs LP$(A(t), b(t), c(t))$, where the entries $A_{ij}(t)$, $b_i(t)$ and $c_j(t)$ are definable functions in an o-minimal structure called the *Hardy field*.

A first contribution is to provide a purely geometric characterization of the tropical central path. We have shown that the tropical analytic center is the greatest element of the tropical feasible set. Moreover, any point of the tropical central path is the greatest element of the tropical feasible set intersected with a sublevel set of the tropical objective function.

Thanks to this characterization, we identify a class of path-following interior-point methods which are not strongly polynomial. This class corresponds to primal-dual interior-point methods which iterates in the so-called "wide" neighborhood of the central path arising from the logarithmic barrier. It includes short step, long step as well as predictor-corrector types of interior-point methods. In more details, we establish a lower bound on the number of iterations of these methods, expressed in terms of the number of tropical segments constituting the tropical central path. In this way, we exhibit a family of linear programs with $3d + 1$ inequalities in dimension $2d$ on which the aforementioned interior point methods require $\Omega(2^d)$ iterations. The same family provides a counterexample to Deza, Terlaky and Zinchenko's conjecture, having a total curvature in $\Omega(2^d)$.

A first part of these results is in the preprint [61], further results been presented in [32].

7.4.3. Tropical approach to semidefinite programming

Participants: Xavier Allamigeon, Stéphane Gaubert, Mateusz Skomra.

Semidefinite programming consists in optimizing a linear function over a spectrahedron. The latter is a subset of $\mathbb{R}^n$ defined by linear matrix inequalities, i.e., a set of the form

$$\left\{x \in \mathbb{R}^n : Q^{(0)} + x_1 Q^{(1)} + \cdots + x_n Q^{(n)} \succeq 0\right\}$$

where the $Q^{(k)}$ are symmetric matrices of order m, and $\succeq$ denotes the Loewner order on the space of symmetric matrices. By definition, $X \succeq Y$ if and only if $X - Y$ is positive semidefinite.

Semidefinite programming is a fundamental tool in convex optimization. It is used to solve various applications from engineering sciences, and also to obtain approximate solutions or bounds for hard problems arising in combinatorial optimization and semialgebraic optimization.

A general issue in computational optimization is to develop combinatorial algorithms for semidefinite programming. Indeed, semidefinite programs are usually solved via interior point methods. However, the latter provide an approximate solution in a polynomial number of iterations, provided that a strictly feasible initial solution. Semidefinite programming becomes a much harder matter if one requires an exact solution. The feasibility problem belongs to $\mathsf{NP}_{\mathbb{R}} \cap \mathsf{coNP}_{\mathbb{R}}$, where the subscript $\mathbb{R}$ refers to the BSS model of computation. It is not known to be in NP in the bit model.

We address semidefinite programming in the case where the field $\mathbb{R}$ is replaced by a nonarchimedean field, like the field of Puiseux series. In this case, methods from tropical geometry can be applied and are expected to allow one, in generic situations, to reduce semialgebraic problems to combinatorial problems, involving only the nonarchimedean valuations (leading exponents) of the coefficients of the input.

To this purpose, we first study tropical spectrahedra, which are defined as the images by the valuation of nonarchimedean spectrahedra. We establish that they are closed semilinear sets, and that, under a genericity condition, they are described by explicit inequalities expressing the nonnegativity of tropical minors of order 1 and 2. These results are gathered in the preprint [49].

Then, we show that the feasibility problem for a generic tropical spectrahedron is equivalent to solving a stochastic mean payoff game (with perfect information). The complexity of these games is a long-standing open problem. They are not known to be polynomial, however they belong to the class $\mathsf{NP} \cap \mathsf{coNP}$, and they can be solved efficiently in practice. This allows to apply stochastic game algorithms to solve nonarchimedean semidefinite feasibility problems. We obtain in this way both theoretical bounds and a practicable method which solves some large scale instances. Part of this latter work has been published in the proceedings of the conference ISSAC 2016 [29].

7.5. Applications

7.5.1. Geometry of the Loewner order and application to the synthesis of quadratic invariants in static analysis of program

Participants: Xavier Allamigeon, Stéphane Gaubert, Nikolas Stott.

This work is in collaboration with Éric Goubault and Sylvie Putot (from LIX).

We introduce a new numerical abstract domain based on ellipsoids designed for the formal verification of switched linear systems. The novelty of this domain does not consist in the use of ellipsoids as abstractions, but rather in the fact that we overcome two key difficulties which so far have limited the use of ellipsoids in abstract interpretation. The first issue is that the ordered set of ellipsoids does not constitute a lattice. This implies that there is a priori no canonical choice of the abstraction of the union of two sets, making the analysis less predictable as it relies on the selection of good upper bounds. The second issue is that most recent works using on ellipsoids rely on LMI methods. The latter are efficient on moderate size examples but they are inherently limited by the complexity of interior point algorithms, which, in the case of matrix inequality problems, do not scale as well as for linear programming or second order cone programming problems.

We developed a new approach, in which we reduce the computation of an invariant to the determination of a fixed point, or eigenvector, of a non-linear map that provides a safe upper-approximation of the action induced by the program on the space of quadratic forms. This allows one to obtain invariants of systems of sized inaccessible by LMI methods, at the price of a limited loss of precision. A key ingredient here is the fast computation of least upper bounds in Löwner ordering, by an algebraic algorithm. This relies on the study of the geometry of the space of quadratic forms (Section 7.2.3).

A first part of this work is described in the article [16], which is the extended version of [65] which won the best paper award at the conference EMSOFT 2015. Followup work is dealing with the extension of these results to switched affine systems with guards.

7.5.2. Performance evaluation of an emergency call center based on tropical polynomial systems

Participants: Xavier Allamigeon, Vianney Boeuf, Stéphane Gaubert.

This work arose from a question raised by Régis Reboul from Préfecture de Police de Paris (PP), regarding the analysis of the projected evolution of the treatment of emergency calls (17-18-112). This work benefited from the help of LtL Stéphane Raclot, from Brigade de Sapeurs de Pompiers de Paris (BSPP). It is part of the PhD work of Vianney Bœuf, carried out in collaboration with BSPP.

We introduced an algebraic approach which allows to analyze the performance of systems involving priorities and modeled by timed Petri nets. Our results apply to the class of Petri nets in which the places can be partitioned in two categories: the routing in certain places is subject to priority rules, whereas the routing at the other places is free choice.

In [62], we introduced a discrete model, showing that the counter variables, which determine the number of firings of the different transitions as a function of time, are the solutions of a piecewise linear dynamical system. Moreover, we establish that in the fluid approximation of this model, the stationary regimes are precisely the solutions of a set of lexicographic piecewise linear equations, which constitutes a polynomial system over a tropical (min-plus) semifield of germs.

In essence, this result shows that computing stationary regimes reduces to solving tropical polynomial systems. Solving tropical polynomial systems is one of the most basic problems of tropical geometry. The latter provides insights on the nature of solutions, as well as algorithmic tools. In particular, the tropical approach allows one to determine the different congestion phases of the system.

We applied this approach to a case study relative to the project led by Préfecture de Police de Paris, involving BSPP, of a new organization to handle emergency calls to Police (number 17), Firemen (number 18), and untyped emergency calls (number 112), in the Paris area. We initially introduced, in [62], a simplified model of emergency call center, and we concentrated on the analysis of an essential feature of the organization: the two level emergency procedure. Operators at level 1 initially receive the calls, qualify their urgency, handle the non urgent ones, and transfer the urgent cases to specialized level 2 operators who complete the instruction. We solved the associated system of tropical polynomial equations and arrived at an explicit computation of the different congestion phases, depending on the ratio of the numbers of operators of level 2 and 1.

We subsequently developed a more complex model, taking into account the different characteristics of the calls to 17 and 18, and developed a realistic simulation tool to validate the results. Moreover, in [28], we developed an alternative model, relying on fluid Petri nets (dynamical systems with piecewise affine vector fields). We showed that the fluid and discrete models have the same stationary regimes, and that some pathological features of the discrete model (anomalous periodic orbits appearing under certain arithmetical conditions) vanish in the fluid Petri net case.

7.5.3. Smart Data Pricing

Participants: Marianne Akian, Jean-Bernard Eytard.

This work is in collaboration with Mustapha Bouhtou (Orange Labs).

The PhD work of Jean-Bernard Eytard concerns the optimal pricing of data trafic in mobile networks. We developed a bilevel programming approach, allowing to an operator to balance the load in the network through price incentives. We showed that a subclass of bilevel programs can be solved in polynomial time, by combining methods of tropical geometry and of discrete convexity. This work has been presented in [31].

ANJA Team

6. New Results

6.1. Legal aspects of systems designed to judicial risk quantification

Participants : Jérôme Dupré

Within the ANJA team systems designed to calculate judicial risk using machine learning technology (AI) have been developed. A former French magistrate is one of the team member who has participated to these researches. In the meantime, he endeavored to contribute to design a legal framework applicable to this activity.

Artificial intelligence (AI), particularly when applied to justice, is liable to encounter rules of law, which are applicable even in the absence of a specific law. As with any new field of activity (eg the Internet), the notion of “legal vacuum” must not be confused with that of “legislative void”. It is therefore necessary to identify how to protect these technologies, what is the responsibilities of each, whether designer or / and user, that could already be applicable.

The two main concerns are relating to property and liability.

1.Regarding property, one can observe that predictive/quantitative solutions based on artificial intelligence result from a combination of technical criterion, databases, algorithms and software, each subject to specific legal protections. These elements may hence be protected by the copyright (for technical criterion); the database law, copyright and unfair competition (for databases); the trade secret (for algorithms), the copyright (for software). It may be questioned whether it would be irrelevant to create, ultimately, a unified legal status specific to this complex reality. But it is probably too early to legislate.

At the heart of the solution is the algorithm, an immaterial element which, in France, is the least well protected by law (it belongs to the domain of “ideas”), justifying its secret nature.

2. Considering liability aspects, we observe that this “black box” - the secret being a consequence of complexity and investments made - may be at the origin of a prejudice, either because of a bad use, or because it is not correctly designed.

The French law offers a range of solutions to the victim, depending on the origin of the damage (see 6.2).

Trust in results is also a factor to be considered. Thus, in the absence of a technical problem peculiar to the solution, misuse by the legal professional providing legal advice may justify, for example, his/her contractual liability. From this standpoint, the reliance granted to the technology and the way it is presented are essential. It justifies a specific attention to the way contracts relating to these services are drafted.

The designer of a defective solution may be required to guarantee against the hidden defects of Article 1641 of the French Civil Code. (When there is no contract, one can also be liable on the grounds of Article 1242 paragraph 1 of the same Code).

Standardization of algorithms, which could be tested by an independent body and subject to secrecy, is also an option, but presents a risk of possible paralysis of a promising market in the field of mathematics.

More generally, it seems necessary to comply with the CNIL (the French Data Protection Authority) provisions relating to personal data (Law No 78-17 of 6 January 1978, spec. article 10, and soon Regulation EU 2016/679 of the European Parliament and of the Council of 27 April 2016 applicable in 2018) and with Privacy Law... A huge amount of data is indeed likely to reveal information not resulting from each data taken separately. But this risk is probably more present in the field of big data than in algorithms, the data used for learning being "dissolved" in the formula.

6.2. Liability and ethics

Participants : Jacques Lévy Véhel, Jérôme Dupré

Some legal issues are specifically related to the calculation error. The system user may not have entered the data correctly and then will be responsible for the displayed result (but it is possible to display the entered data with the results to limit this risk).

The user may also have entered the data correctly and: -he/she is aware of the error of the system, in which case the user regains a share of responsibility, -he/she is not aware of the error of the system and the error is not easily detectable, then the responsibility should move towards the authors of the system conception (with its different steps that result from each other: definition of the search criteria, creation of database and creation of the algorithm, development and integration of the software, etc.). -he/she is not aware of the error of the system and the error is easily detectable, in which case the user should regain at least some responsibility.

The use of systems designed to judicial risk quantification entails paradigm shift The probabilistic approach, where all things are equal, seems very far from the hierarchy of legal norms and legal causality. In the absence of any upheaval in the law, we can at least expect an upheaval in legal practice.

Ultimately, the use of predictive tools, which favors the discovery of correlations, may lead to less attention to the causes of events, hence the need to maintain a vigilance on this aspect. The human who "delegates everything" to the machine should not avoid responsibility.

From an ethical perspective, is it acceptable to calculate the sentence which is likely to be pronounced in penal law, e.g. for a crime? Should we accept to profile judges using all their past rulings?

More generally, a reflection as well as a study on the place left to the human at all the stages of the process of elaboration and use (the decision-making) of the predictive tools seems necessary.

6.3. Statistical inference methods for panel of random-coefficient AR(1) data

Participants: A. Philippe and D. Surgailis R. Leipus and V. Pilipauskaitė (Vilnius university)

We study the statistical inference methods for panel of random-coefficient AR(1) data [17] . We propose a nonparametric estimation of the distribution function of random coefficients by the empirical distribution of lag 1 sample correlations of individual AR(1) processes. Consistency and asymptotic normality of the empirical distribution function and a class of kernel density estimators is established under some regularity conditions on G(x) as N and n increase to infinity. An extension of this work consists in testing the presence of long memory. The procedure is based on the tail index of G and the théorie of extreme values. In the same direction, a new frequency-domain test statistic is introduced to test for short memory versus long memory, see [23]

6.4. New Bayesian approach for chronological modeling

Participants: Anne. Philippe and Marie-Anne Vibet in collaboration with IRAMAT - Université Bordeaux Montaigne

We have been working on the construction of new Bayesian approach for chronological modeling: this is an important issue in archaeology and paleo-environmental sciences. The proposed solution is based on the "event model'. We define the Event as the date of an archeological context determined from a collection of contemporaneous artifacts. We obtain a robust approach with respect to outliers due to the sampling in the field or the measurement process in the laboratory.

In [25] We propose new tools to analyse the chronologies especially regarding phases. They are implemented in R package 'RChronoModel'.

In [22], [18], [5], we propose bayesian models for optically stimulated luminescence dating. It consists in estimating a central equivalent dose from a set of luminescence measurements. Then a calibration step is required to convert equivalent dose into calendar date.

6.5. Self-regulated processes

Participants : Jacques Lévy Véhel, Anne Philippe, Caroline Robet

We wish to construct various instances of processes Z such that, at each point t, almost surely, the pointwise Hölder exponent of Z at t, denoted $\alpha_Z(t)$, verifies

$$\alpha_Z(t) = g(Z(t))$$

where $g \in \mathcal{C}^1(\mathbb{R}, [a, b])$ is a deterministic function. Then, we would estimate the function g which control the regularity.

The pointwise Hölder exponent at t of a function or a process $f : \mathbb{R} \to \mathbb{R}$, which is $\mathcal{C}^1$ nowhere, is the real $\alpha_f(t)$ such that :

$$\alpha_f(t) = \sup\{\beta, \limsup_{h \to 0} \frac{| f(t+h) - f(t) |}{| h |^\beta} = 0\}$$

We worked first on pathwise integrals :

Theorem 1 Let $g \in \mathcal{C}^1(\mathbb{R}, [a, b])$, $0 < a < b < 1$. Provided $\|g'\|_\infty$ is small enough, there exists a unique continuous process Z verifying almost surely on $[0, T]$

$$Z_t = \int_0^t (t-u)^{g(Z_u)-1} W_u \, du$$

where W is an almost surely continuous process.

A random condition ($\|g'\|_\infty \|W(\omega)\|_\infty C(a, T) < 1$) appears in the application of Banach fixed point theorem (in $(\mathcal{C}^0([0, T]; \mathbb{R}), \|.\|_\infty)$). It implies that it is possible to have existence et uniqueness only on $[0, t']$, $t' < T$. We simulated pathwise integrals and showed some cases without uniqueness. We studied some easier processes in order to find the regularity of Z.

Theorem 2 Let $h \in]0, 1[$ and U defined on $[0, T]$ by

$$U_t = \int_0^t (t-u)^{h-1} W_u \, du$$

Then $\forall t \in [0, T]$, $\alpha_U(t) \geq h$.

Theorem 3 Let $g \in \mathcal{C}^1(\mathbb{R}, [a, b])$, $0 < a < b < 1$. Provided $\|g'\|_\infty$ is small enough, there exists a unique continuous process Y verifying almost surely on $[0, T]$

$$Y_t = \int_0^t (t-u)^{g(Y_t)-1} W_u \, du$$

where W is an almost surely continuous process. Furthermore, $\forall t \in [0, T]$, $\alpha_Y(t) \geq g(Y_t)$

Then, we adapted the multifractional Brownian Motion [50], [31] (which a representation is $B_t = \int_0^t K_{H(t)}(t, u) W(du)$, W Brownian Motion et H$\in \mathcal{C}^1$) to construct the modified multifractional Brownian Motion : $Z_t = \int_0^t K_{H(u)}(t, u) W(du)$. We expect obtain a self-regulated process $Y_t = \int_0^t K_{g(Y_u)}(t, u) dW(u)$.

Theorem 4 Let $g \in \mathcal{C}^1(\mathbb{R}, [a, b])$, $0 < a < b < 1$. Provided $\|g'\|_\infty$ is small enough, there exists a unique continuous adapted process Y include in $\mathcal{C}^0([0, T]; L^2(\Omega))$ verifying almost surely on $[0, T]$

$$Y_t = \int_0^t K_{g(Y_u)}(t, u) dW(u)$$

where W is the Brownian motion.

6.6. Causal inference by independent component analysis with Application of to American macro-economic data

Participants : Jacques Lévy-Vehel, Anne Philippe, Marie-Anne Vibet

The aim of this work is to study the causal relationships existing among macro-economic variables under investigation, and trace out how economically interpreted random shocks affect the system. Structural vector of autoregressive models (SVAR) are usually applied in this kind of study and the causal structure is driven by the data. In this work, independent component analysis (ICA) is implemented in order to guaranty the identifiability of the causal structure. However, the use of ICA can only be done under the hypothesis that the residuals are non-Gaussian, an hypothesis easily verified with economic data.

The vector of autoregressive (VAR) model has the following reduced representation :

$$Y_t = A_1 Y_{t-1} + ... + A_p Y_{t-p} + u_t \text{ , for } t = 1, ..., T$$

where, Y_t, is the vector of contemporaneous variables of dimension $K \times 1$, p is the number of autoregressive variables, A_j, for $j = 1, ..., p$, are matrices of dimension $K \times K$ estimated by the model and u_t is the vector of random disturbances of dimension $K \times 1$ and assumed to be a zero-mean white noise process, $u_t \sim N(0_K, \Sigma_u)$. Given enough data, both Σ_u and all matrices A_j can be corretly estimated by the VAR model.

However, the VAR model is not sufficient for policy analysis. Indeed, using the Moving Average representation of a stable VAR :

$$Y_t = \sum_{j=0}^{\infty} \Phi_j u_{t-j} \tag{9}$$

where $\Phi_0 = I_K$ and $\Phi_j, j \geq 1$, are the coefficients matrices representing the impulse responses of the elements of Y_t to the disturbances u_{t-j}. This representation is not unique.

The structiral VAR (SVAR) is essentially a VAR equipped with a particular choice of a matrix P so that $Y_t = \sum_{j=0}^{\infty} \Phi_j P P^{-1} u_{t-j} = \sum_{j=0}^{\infty} \Psi_j \epsilon_{t-j}$

where ϵ_{t-j} are independent random shocks economically interpreted. To this aim, the ICA procedure is then used to find the proper matrix P using the hypothesis that the residuals, ϵ_{t-j}, are non-Gaussian.

We used the VAR-LINGAM procedure developped by Moneta *et al* [28] and their package written for R software. We started by testing this procedure with a series of simulations study. We tackled the following questions : Are the coefficients of the matrices B and A well estimated by the VARLINGAM procedure ? Is the bootstrap function appropriate, and in particular, does it estimate properly the standard error of the coefficients of matrices A and B ? And how long should the economic data be in order to estimate correctly the coefficients of the matrices B ?

As the conclusion to all these studies were correct enough, we went on analysing our real data that consists of 6 weekly time series US macro-economic data, reported from the first week of January 1996 to April 2016 : The BofA Merrill Lynch US Broad Market Index, The Bofa Merril Lynch US Corporate Index, Equity Indices S&P, 500, Federal Funds Rates,Treasury Bills, Other Factors Draining Reserve Balances.

The conclusions of this work is in discussion with economists and a paper will soon be written.

6.7. SAR image denoising using an irregularity-preserved denoising technique based on the global Höllder exponent

Participants : Jacques Lévy-Vehel, Yue Huang

This work addresses the speckle noise reduction for SAR images by using the irregularity-preserved denoising technique proposed in [34]. This irregularity preserving denoising scheme in [34] may be summarized as a three-step process in the following:

1. Apply a Discrete Wavelet Transform (DWT) on the noisy signal and represent the resulting coefficients distribution over scales. Estimate the cut-off scale and the global Hölder exponent α_f using linear regression of $\max_k \left(\log_2 |\langle f, \psi_{j,k} \rangle| \right)$ at larger scales.
2. Extrapolate the larger scale regression line to smaller scales and limit coefficient at smaller scales ($j \geq j_{\text{cut-off}}$) to the boundary value obtained from the linear regression
3. Reconstruct the filtered signal from the set of modified coefficients

where f is the signal under analysis, $\psi_{j,k}$ is the wavelet basis, and $\langle f, \psi_{j,k} \rangle$ is the wavelet coefficient of f at scale j and location k. As it has been shown by simulations in [34], to retrieve irregular signals affected by additive noise, this technique outperforms conventional denoising techniques that apply hard or soft thresholding to the wavelet coefficients.

Considering a speckle-affected SAR image, a complex SAR signal may be represented by:

$$y(l) = s(l)u(l)$$

where l represents one of L realizations, and the noise term $u(l)$ follows a complex circular centered Gaussian white distribution with unit variance, i.e. $u \sim \mathcal{N}_C(0,1)$, $E(u(i)u^*(j)) = \delta_{(i-j)}$. The texture of SAR image significantly depends on the backscattering power $\sigma(l) = |y(l)|^2$.

We aim to use the irregularity-preserved denoising technique to denoise SAR image and enhance its texture. We tested firstly on the simulated signals affected by multiplicative noise and then on real SAR images. This denoising scheme showed potential to reduce the speckle noise, preserve the irregularity of image texture and enhance target signature.

Although the results have been compared with other SAR speckle filtering techniques, we still need more efforts for validation. As long as the results are validated, the work will be written in a paper.

6.8. Underfoliage object imaging using SAR tomography and wavelet-based sparse estimation methods

Participants : Yue Huang, Jacques Lévy-Vehel

Hybrid environments refer to a scenario of deterministic objects embedded in a host natural random environment and their scattering patterns consist of a complex mixture of diverse mechanisms, like, in the case of this study, volume scattering from the canopy, double bounce reflection between the ground and under-foliage objects as well as between objects and trunks, surface scattering from the underlying ground, etc. The resulting SAR information is characterized by a strong complexity, and its analysis using 2-D images or even data acquired in InSAR configuration remains difficult. Using Multi-baseline(MB) InSAR data, SAR tomography can be applied to reconstruct in 3-D the measured scattering responses and polarimetric patterns. Natural volumes, such as forest canopies, being composed of a large number of scatterers whose responses cannot be discriminated at the resolution of analysis, their scattering patterns are generally considered as a vertical density of random or speckle-affected reflectivity. On the other hand, localized objects, such as artificial targets on the ground are associated to point-like contributions, that may be separable in the vertical direction. The global response of under-foliage objects with a deterministic scattering response embedded in surrounding distributed environments, can be described by a mixed spectrum. Conventional tomographic techniques like the Capon and Beamforming methods, estimate continuous Power Spectral Density (PSD) and hence are well adapted to the characterization of continuous volumetric media, but cannot discriminate closely-spaced scatterers, e.g. scattering responses from trucks, due to limited spatial resolution. Conventional high-resolution methods like MUSIC and subspace fitting estimators as well as sparse estimation techniques such as LASSO

[52] and FOCUSS [40], are well adapted to the characterization of discrete scatterers like truck top, truck-ground interaction and calibrators over bare soils, or buildings over urban areas [53], but cannot properly handle the high dimensionality of the scattering responses of natural volumes. Usual tomographic techniques cannot simultaneously cope with both types of spectrum, and not able to deal with mixed spectral estimation problems, characteristic of underfoliage object imaging scenario.

Wavelet-based techniques present a high potential for such applications, as they permit to parameterize in a sparse way continuous functions, i.e. canopy PSDs in the present case. Wavelet-based tomographic techniques have been used for tomographic imaging of forested areas [27], and for such regular signals, large wavelet coefficients being often concentrated in the approximation space, scale thresholding may be implemented to extract the most significant wavelet coefficients for an accurate volume signal recovery [27]. In the underfoliage object scenario, discrete scatterers embedded in a continuous medium, result in a mixed vertical PSD that may be associated to an irregular signal with wavelet coefficients distributed both in the approximation and detail spaces, and a simple scale cut-off is hence not adapted to separate the wavelet coefficients of discrete scatterers from those of continuous media. Therefore, we propose a new wavelet-based method to extract underfoliage objects from their speckle-affected distributed environment and characterize them with a high resolution.

For an MB-InSAR configuration with M acquisition positions, considering an azimuth-range resolution cell containing a mixture of backscattering contributions from object (o) and volume (v) scatterers located at different heights z, the observed data vector at lth realization can be represented by:

$$\mathbf{y}(l) = \mathbf{A}_o(\mathbf{z}_o)\mathbf{s}_o(l) + \mathbf{A}_v(\mathbf{z}_v)\mathbf{s}_v(l) + \mathbf{n}(l) \tag{10}$$

where the steering matrix, $\mathbf{A}_x(\mathbf{z}_x)$, contains the interferometric phase information associated to the InSAR responses of the scatterers located at the unknown elevation positions $\mathbf{z}_x = [z_{x_1}, \cdots, z_{x_{N_x}}]$ above the reference focusing plane, and the source signal vector, $\mathbf{s}_x = [s_{x_1} \cdots s_{x_{N_x}}]^T \in \mathbb{C}^{N_x \times 1}$, contains the unknown complex backscattering coefficients of the N_x source scatterers. The vertical reflectivity function can be represented as $\mathbf{p}_x = E(|\mathbf{s}_x|^2)$ $(x = o, v)$.

Over speckle-affected environments, unknown reflectivity and elevation parameters are generally estimated from second-order statistics, i.e. from the covariance matrix $\widehat{\mathbf{R}} \in \mathbb{C}^{M \times M}$ of the observed MB-InSAR data $\mathbf{y} \in \mathbb{C}^{M \times 1}$. The proposed tomographic processing technique is based on the minimization of the Least-Square (LS) fitting between the observed and modeled data covariance $||\mathbf{R} - \widehat{\mathbf{R}}||_F$. The modeled covariance matrix is composed by the covariances of object and volume contributions $\mathbf{R} = \mathbf{R}_o + \mathbf{R}_v$, each of them being simply related to its discretized vertical density of reflectivity $\mathbf{p}_x$ through $\mathbf{R}_x = \mathbf{A}(\mathbf{z}_x)\,\mathrm{diag}\,(\mathbf{p}_x)\mathbf{A}^H(\mathbf{z}_x) \in \mathbb{C}^{M \times M}$. The proposed method can be represented by a l_1 norm minimization in a transformed space subject to quadratic constraints between the observed and modeled data covariance:

$$\min_{\mathbf{p}} ||\mathbf{B}\mathbf{p}||_1 \text{ subject to } \quad ||\mathbf{R} - \widehat{\mathbf{R}}||_F \leq \epsilon \tag{11}$$

where

- $\mathbf{p} = [\mathbf{p}_o^T \quad \mathbf{p}_v^T]^T \in \mathbb{R}^{+N_s \times 1}$ stands for vertical backscattering power distribution for the resolution cell under analysis,
- $\mathbf{B} = \begin{bmatrix} \mathbf{I}_{(N_o \times N_o)} & \mathbf{0} \\ \mathbf{0} & \Psi_{(N_v \times N_v)} \end{bmatrix} \in \mathbb{R}^{(N_s \times N_s)}$ represents the hybrid sparsifying basis with the wavelet basis Ψ

This tomographic technique is suitable for the mixed-spectrum estimation problem, because it maintains the spectral continuity for the backscattering power of forest canopies and the high-resolution for the vertical reflectivity of objects. The effectiveness of this new approach is demonstrated using L-band airborne tomographic SAR data aquired by the DLR over Dornstetten, Germany. The undeniable performance can be shown by the results in [21] and [20].

This work has been presented in European SAR conference 2016 . Some refined results have been presented in IGARSS conference 2016 as an invited talk. By extending this work in details, a journal paper [24] has been submitted to IEEE Geoscience and Remote Sensing Letters (GRSL) and is currently under reviewing.

6.9. Detection of objects concealed beneath forest canopies using Time-Frequency techniques

Participants : Yue Huang, Jacques Lévy-Vehel

In the scenario of hybrid environments where objects with a deterministic response are embedded in a speckle affected environment, the parameter estimation for this type of scatterers becomes a problem of mixed-spectrum estimation. To isolate and characterize these different scattering contributions, a novel method proposed by Huang et al. was used to extract isolated scatterers (IS) from their surrounding distributed environments, named IS extraction in [42]. Incorporating the Weighted Subspace Fitting (WSF) estimator, this method estimated scattering responses within one resolution cell and then distinguishes isolated scatterers from distributed ones by calculating the cross-correlation between the measured data and the estimated scattering responses. Moreover, to compare the detection performance for coherent scatterers, two statistical methods have been applied to analyse hybrid environments in [43]: GLRT (generalized likelihood ratio test)-based and SSF (weighted Signal Subspace Fitting)-based detection procedures. However, the above mentioned methods based on discrete high-resolution tomographic estimation, require to preselect the number of scattering contributions, which may induce reliability issues due to model order selection.

This paper proposes a new tomographic estimator based on Time-Frequency (TF) techniques using Multi-baseline Polarimetric and Interferometric SAR data. The coherent TF analysis of polarimetric SAR has been introduced in [38], [39] for the study of anisotropic scattering behaviors and then applied in [37], [36] for dense urban environment characterization. Time-frequency techniques can represent spectral properties around specific spatial locations or spatial features at specific spectral positions, leading to describe local variations of spectral or spatial features. Considering SLC SAR images, the spectral locations can be linked to azimuth looking angle and illumination frequency in such a way:

$$w_{az} = \frac{4\pi}{c} f_c v_{SAR} \sin\phi, \quad w_{rg} = \frac{4\pi}{c}(f - f_c)$$

with f_c central frequency and ϕ azimuth looking angle. The TF technique can be used to analyze scattering behaviors at different illuminated positions and frequency components during SAR integration. Based on the correlation between different spectral positions, the TF indicator proposed in [37] can extract coherent components in complex random SAR responses. Polarimetric TF indicator has been developed in [41] for ship discrimination. In this paper, the new tomographic estimator extends 2-D TF analysis to 3-D, which provides an efficient cancellation for clutters from speckle-affected random scattering environments, and discriminates the deterministic responses from coherent scatterers in 3-D space. The effectiveness of this new tomographic approach is demonstrated by using L-band MB-PolInSAR data set acquired over the test site of Dornstetten where the underfoliage objects are set up. The fully polarimetric version of this TF tomographic estimator is also developed to improve the detection efficiency. This work has been accepted for oral presentation at the Polinsar 2017 Workshop and the final paper will be written by the end of Workshop.

DOLPHIN Project-Team

7. New Results

7.1. Optimization under uncertainty

Participants: El-Ghazali Talbi, Raca Todosijevic, Oumayma Bahri (externel collaborators: Nahla BenAmor - Univ. Tunis, Tunisia, J. Puente, C. R. Vela, I. Gonzalez-Rodriguez - Univ. Oviedo Spain)

At the problem level, the sources of uncertainty are due to many factors such as the environment parameters of the model, the decision variables and the objective functions. Examples of such uncertainties can be the demand and travel times in vehicle routing problems, the execution time in scheduling problems, the wind or solar production in energy power systems, the price of resources in manufacturing, and the mechanical properties of a structure. Then, we need precise and efficient modeling and resolution approaches which are robust and non-sensitive to those uncertainties. The appeal of optimization under uncertainty is that its performance results remain relatively unchanged when exposed to uncertain data.

We have considered the fuzzy job shop, a job shop scheduling problem with uncertain processing times modelled as triangular fuzzy numbers. While the usual approaches to solving this problem involve adapting existing metaheuristics to the fuzzy setting, we have proposed instead to follow the framework of simheuristics from stochastic optimisation. More precisely, we integrate the simulation of possible realisations of the fuzzy problem with a genetic algorithm that solves the deterministic job shop. We test the resulting method, simGA, on a testbed of 23 benchmark instances and obtain results that suggest that this is a promising approach to solving problems with uncertainty by means of metaheuristics [38].

7.2. Indicator-based Multiobjective Optimization

Participants: Bilel Derbel, Arnaud Liefooghe (external collaborators: Matthieu Basseur, Adrien Goëffon, Univ. Angers, France)

A large spectrum of quality indicators has been proposed so far to assess the performance of discrete Pareto set approximations in multiobjective optimization. Such indicators assign, to any solution set, a real-value reflecting a given aspect of approximation quality. This is an important issue in multiobjective optimization, not only to compare the performance and assets of different approximate algorithms, but also to improve their internal selection mechanisms. In [37], we adopt a statistical analysis to experimentally investigate by how much a selection of state-of-the-art quality indicators agree with each other for a wide range of Pareto set approximations from well-known two- and three-objective continuous benchmark functions. More particularly, we measure the correlation between the ranking of low-, medium-, and high-quality limited-size approximation sets with respect to inverted generational distance, additive epsilon, multiplicative epsilon, R2, R3, as well as hypervolume indicator values. Since no pair of indicators obtains the same ranking of approximation sets, we confirm that they emphasize different facets of approximation quality. More importantly, our statistical analysis allows the degree of compliance between these indicators to be quantified.

Subset selection constitutes an important stage of any evolutionary multiobjective optimization algorithm when truncating the current approximation set for the next iteration. This appears to be particularly challenging when the number of solutions to be removed is large, and when the approximation set contains many mutually non-dominating solutions. In particular, indicator-based strategies have been intensively used in recent years for that purpose. However, most solutions for the indicator-based subset selection problem are based on a very simple greedy backward elimination strategy. We experiment additional heuristics that include a greedy forward selection and a greedy sequential insertion policies, a first-improvement hill-climbing local search, as well as combinations of those. We evaluate the effectiveness and the efficiency of such heuristics in order to maximize the enclosed hypervolume indicator of candidate subsets during a hypothetical evolutionary process, or as a post-processing phase. Our experimental analysis, conducted on randomly generated as well as structured two-, three- and four-objective mutually non-dominated sets, allows us to appreciate the benefit of these approaches in terms of quality, and to highlight some practical limitations and open challenges in terms of computational resources.

7.3. Decomposition-based Multiobjective Optimization

Participants: Bilel Derbel, Arnaud Liefooghe (external collaborators: Hernan Aguirre and Kiyoshi Tanaka, Shinshu Univ., Japan; Qingfu Zhang, City Univ., Hong Kong)

It is generally believed that local search (LS) should be used as a basic tool in multi-objective evolutionary computation for combinatorial optimization. However, not much effort has been made to investigate how to efficiently use LS in multi-objective evolutionary computation algorithms. In [28], we study some issues in the use of cooperative scalarizing local search approaches for decomposition-based multiobjective combinatorial optimization. We propose and study multiple move strategies in the MOEA/D framework. By extensive experiments on a new set of bi-objective traveling salesman problems with tunable correlated objectives, we analyze these policies with different MOEA/D parameters. Our empirical study has shed some insights about the impact of the Ls move strategy on the anytime performance of the algorithm.

7.4. Learning and Adaptation for Landscape-aware Algorithm Design

Participants: Bilel Derbel, Arnaud Liefooghe (external collaborators: Hernan Aguirre, Fabio Daolio, Miyako Sagawa and Kiyoshi Tanaka, Shinshu Univ., Japan; Cyril Fonlupt, Christopher Jankee and Sébastien Verel, Univ. Littoral, France)

In [13], we attempt to understand and to contrast the impact of problem features on the performance of randomized search heuristics for black-box multi-objective combinatorial optimization problems. At first, we measure the performance of two conventional dominance-based approaches with unbounded archive on a benchmark of enumerable binary optimization problems with tunable ruggedness, objective space dimension, and objective correlation (ρMNK-landscapes). Precisely, we investigate the expected runtime required by a global evolutionary optimization algorithm with an ergodic variation operator (GSEMO) and by a neighborhood-based local search heuristic (PLS), to identify a $(1 + \varepsilon)$-approximation of the Pareto set. Then, we define a number of problem features characterizing the fitness landscape, and we study their intercorrelation and their association with algorithm runtime on the benchmark instances. At last, with a mixed-effects multi-linear regression we assess the individual and joint effect of problem features on the performance of both algorithms, within and across the instance classes defined by benchmark parameters. Our analysis reveals further insights into the importance of ruggedness and multi-modality to characterize instance hardness for this family of multi-objective optimization problems and algorithms.

Designing portfolio adaptive selection strategies is a promising approach to gain in generality when tackling a given optimization problem. However, we still lack much understanding of what makes a strategy effective, even if different benchmarks have been already designed for these issues. In [35], we propose a new model based on fitness cloud allowing us to provide theoretical and empirical insights on when an on-line adaptive strategy can be beneficial to the search. In particular, we investigate the relative performance and behavior of two representative and commonly used selection strategies with respect to static (off-line) and purely random approaches, in a simple, yet sound realistic, setting of the proposed model.

In evolutionary multi-objective optimization, variation operators are crucially important to produce improving solutions, hence leading the search towards the most promising regions of the solution space. In [39], we propose to use a machine learning modeling technique, namely random forest, in order to estimate, at each iteration in the course of the search process, the importance of decision variables with respect to convergence to the Pareto front. Accordingly, we are able to propose an adaptive mechanism guiding the recombination step with the aim of stressing the convergence of the so-obtained offspring. By conducting an experimental analysis using some of the WFG and DTLZ benchmark test problems, we are able to elicit the behavior of the proposed approach, and to demonstrate the benefits of incorporating machine learning techniques in order to design new efficient adaptive variation mechanisms.

7.5. Feature Selection using Tabu Search with Learning Memory: Learning Tabu Search

Participants: C. Dhaenens, L. Jourdan, M-E. Kessaci

Feature selection in classification can be modeled as a combinatorial optimization problem. One of the main particularities of this problem is the large amount of time that may be needed to evaluate the quality of a subset of features. We propose to solve this problem with a tabu search algorithm integrating a learning mechanism. To do so, we adapt to the feature selection problem, a learning tabu search algorithm originally designed for a railway network problem in which the evaluation of a solution is time-consuming. Experiments conducted show the benefit of using a learning mechanism to solve hard instances of the literature [hal-01370396v1].

7.6. MO-ParamILS: A Multi-objective Automatic Algorithm Configuration Framework

Participants: C. Dhaenens, L. Jourdan, M-E. Kessaci

Automated algorithm configuration procedures play an increasingly important role in the development and application of algorithms for a wide range of computationally challenging problems. Until very recently, these configuration procedures were limited to optimising a single performance objective, such as the running time or solution quality achieved by the algorithm being configured. However, in many applications there is more than one performance objective of interest. This gives rise to the multi-objective automatic algorithm configuration problem, which involves finding a Pareto set of configurations of a given target algorithm that characterises trade-offs between multiple performance objectives. In this work, we introduced MO-ParamILS, a multiobjective extension of the state-of-the-art single-objective algorithm configuration framework ParamILS, and demonstrated that it produces good results on several challenging bi-objective algorithm configuration scenarios compared to a base-line obtained from using a state-of-the-art single-objective algorithm configurator. [hal-01370392].

7.7. Parallel optimization methods revisited for multi-core and many-core (co)processors

Participants: J. Gmys and N. Melab

This contribution is a joint work with M. Mezmaz, E. Alekseeva and D. Tuyttens from University of Mons (UMONS) and T. C. Pessoa and F. H. De Carvalho Junior from Universidade Federal Do Cearà (UFC), Brazil. On the road to exascale, coprocessors are increasingly becoming key building blocks of High Performance Computing platforms. In addition to their energy efficiency, these many-core devices boost the performance of multi-core processors. During 2016, we first have revisited the design and implementation of parallel Branch-and-Bound (B&B) algorithms using the work stealing paradigm on GPU accelerators [16][40], multi-GPU systems [17], multi-core processors [15] and MIC (Xeon Phi) coprocessors [20]. The challenge is to take into account the high irregular nature of the B&B algorithm and the hardware characteristics of GPU, Xeon Phi and multi-core (co)processors. Several work stealing strategies have been investigated while addressing several issues: host-device data transfer, thread divergence and data placement on the hierarchy of memories of the GPU and vectorization on Xeon Phi. The proposed approaches have been extensively experimented considering permutation-based optimization problems (e.g. FSP). The results reported in the cited papers demonstrate the efficiency of the many-core approaches compared to their multi-core counterpart. An extension of the proposed approaches to large hybrid clusters, including multi-core and many-core (co)processors is already started in [27].

The second part of the contribution consists in proposing a new hyper-heuristic (generalized GRASP) together with its parallelization for multi-core processors [11]. A cost function based on a bounding operator (used in B&B) is integrated to GRASP for the first time. Multi-core computing is used to investigate 315 GRASP configurations. In order to improve the performance of the local search procedure used in GRASP, we have proposed in [33] an original vectorization of the cost function of the makespan of FSP on Xeon Phi coprocessors. The reported results show that speed-ups up to 4.5 can be achieved compared to a non-vectorized apprpoach.

GEOSTAT Project-Team

6. New Results

6.1. Automatic segmentation of activation periods in an electrogram during atrial fibrillation

Participants: G. Attuel, H. Yahia.

Experiments show that the multiscale properties displayed in signals recording the electrical activity of the heart during (atrial) fibrillation are of the type *out of equilibrium dynamics*. These dynamics have common features, possibily shared by "subclasses": "$1/f$ power spectrum", large proability laws for the distributions of the amplitude increments, multifractal spectra. Theoretically these dynamics are at least the result of a competition between elastic energies and disorder, which leads to the emergence of collective behaviours. Mathematically, the universality classes involved are not those corresponding to the central limit theorem, but generalize it in its more elaborated forms (Levy & Gnedenko). A class has recently been described completely: directed polymers on a random medium. Scaling exponents are known, together with the fluctuations' statistics. Large deviation theory plays a central role. The fixed point of the associated dynamics is that of KPZ (Kardar-Parisi-Zhang). We have indications that heartbeat dynamics in episodes of atrial fibrillation belongs to that class. In such a context, the questions raised relate to finite size effects when asymptotic convergence is slow. From an experimental point of view, the problem of determining universality classes is very hard. However, it is possible to formulate hypothesis on the universality class so as to extract important information from acquisition signals. A good modus operandi consists in using key properties of a model stated *a priori*, to combine them with experimental signal analysis in order to produce *a posteriori* characteristics of interest. Last year, we developed the first model of cardiac dynamics compatible with observed data. The model allows us to test the efficiency of a combined methodology using singularity exponents and Bayesian analysis. This has led us to a first automatic method able to identify periods of cardiac activity and make the distinction with measure noise. From this, the fine automatic determination of activity periods become tractable. This will lead to an automatic quantitative determination of fragmentation, hence opening the way for a determination of universality classes. We illustrate some steps in the figures below.

Publications: [24], [23], [25]

6.2. Pathological voice classification

Participants: K. Daoudi, N. Brodu.

We propose a fully reproducible speech-based technique for objective differential diagnosis between progressive supranuclear palsy (PSP) and multiple system atrophy (MSA). Our technique yields a classification mean accuracy of 86.1% which is a significant improvement as compared to a recent pioneer study on this task. We also show that information extracted through a variety of speech tasks can be used to estimate the degree of Parkinson's disease severity.

Publications: [18], [20], [https://hal.inria.fr/hal-01360038].

6.3. Temporal evolution of coastal upwelling

Participants: A. El Aouni, K. Minaoui, A. Tamim, K. Daoudi, H. Yahia, A. Atillah, D. Aboutajdine.

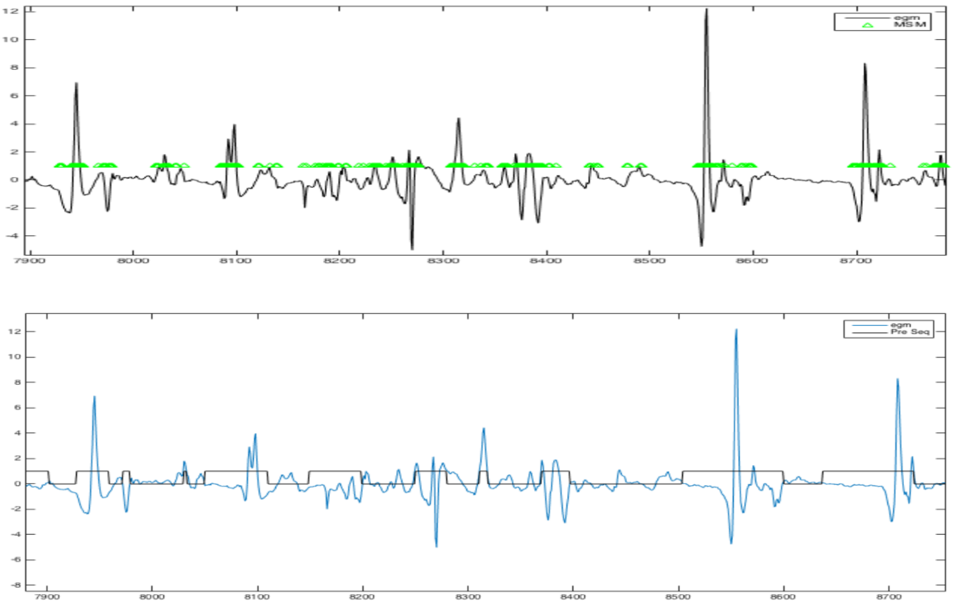


Figure 1. Egm during fibrilllation (in black). Density of the most singular manifold (in green). Result of a 2-state HMM (in blue).

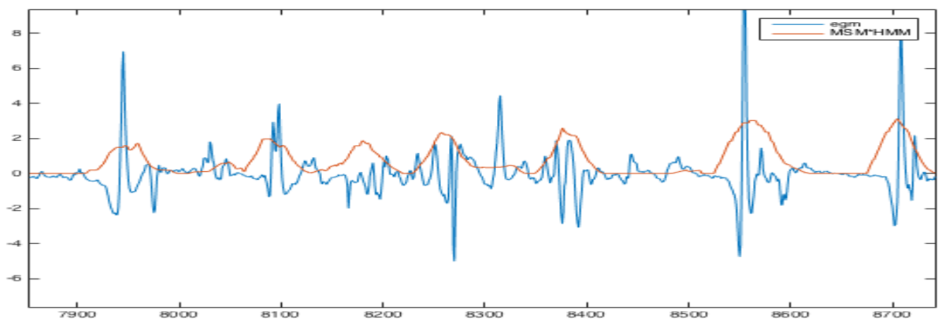


Figure 2. Egm during fibrillation (in blue). Signal of activation probability computed with the result of an HMM and the singularity density (in red).

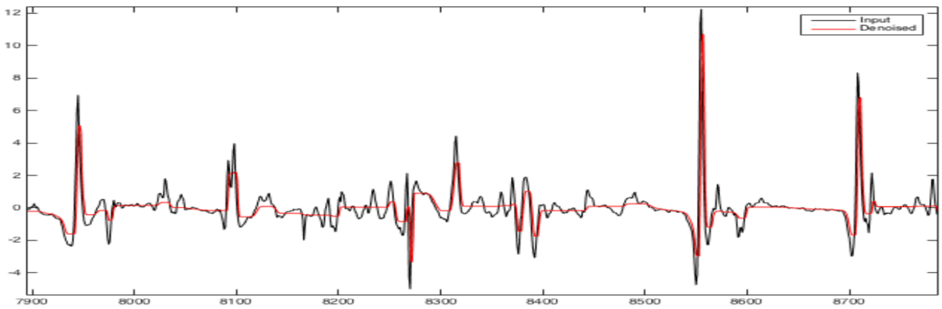


Figure 3. Egm during fibrillation (in black). Signal denosised (norm L^p) (in red).

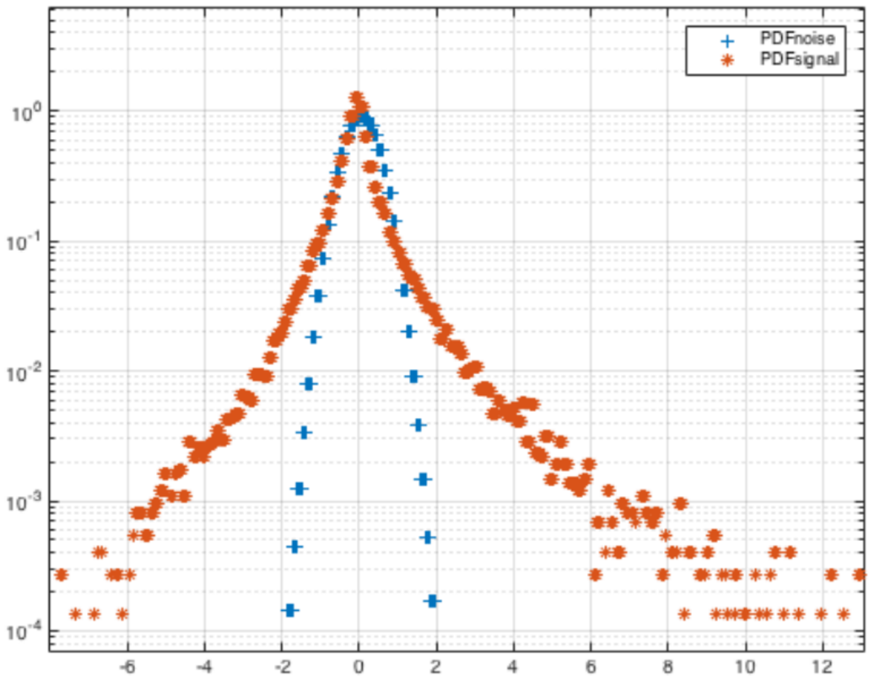


Figure 4. Probability distribution of estimated noise (in blue). Distribution of estimated active dynamics (in red).

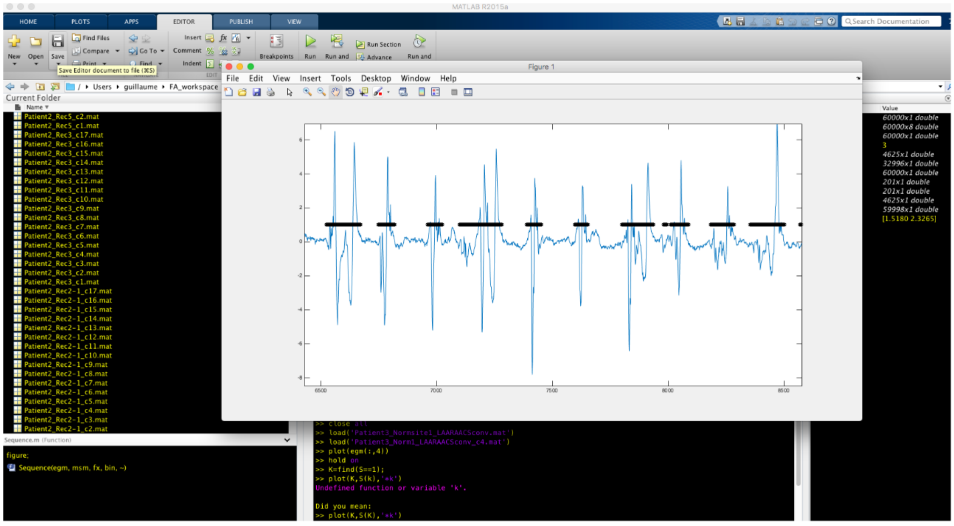


Figure 5. Snapshot of the software (written partially in Matlab and which makes use of FluidExponents). The image shows the result of sequencing, with average confidence level, of a real egm

We present a new methodology to derive rigorous SST-based coastal upwelling index for the purpose of conducting a saisonal variablity of upwelling area along the Moroccan Atlantic coast. The method is based on the scientific knowledge of upwelling area and its spatial dis- tribution provided by expert oceanographers.The latter consists in automatically identify and extract the region covered by the upwelling waters in the costal ocean of Morocco using the Fuzzy c-means algorithm and finding regions of homogeneous pixels. Then Region Growing process is used to filter out the remaining noisy structures in the offshort waters. The methodology is used to provide a satistical view of the spatial and temporal variability of the Moroccan upwelling activity. The relevance of the proposed Coastal Upwelling Index (CUI) is evaluated by an oceanographer using 86 8-days sea surface temperature images and it is shown to be superior to that of the standard upwelling index.
Publication: [https://hal.inria.fr/hal-01424036].

6.4. Non-local and low rank approach for integrability

Participants: H. Badri, H. Yahia.
A formulation is proposed which consists in a sparse gradient data-fitting term to handle outliers together with a gradient-domain non-local low-rank prior.
Publication: [15].

6.5. Low-Rankness transfer for realistic denoising

Participants: H. Badri, H. Yahia, D. Aboutajdine.
Current state-of-the-art denoising methods such as non-local low-rank approaches are mainly tuned to work with uniform Gaussian noise corruption and known variance, which is far from the real noise scenario. Noise level estimation is already a challenging problem and denoising methods are quite sensitive to this parameter. Moreover, these methods are based on shrinkage models that are too simple to reflect reality, which results in over-smoothing of important structures such as small-scale text and textures. We propose a new approach for more realistic image restoration based on the concept of low-rankness transfer (LRT).

Publication: [14].

6.6. Multiscale methods for Earth Observation data

Participants: H. Yahia, N. Brodu, V. Garçon, J. Sudre, S. Kumar Maji, D. Singh, K. Daoudi, D. Aboutajdine.
Earth observation data of different kinds are tested for super-resolution or analysis using the multiscale approaches developped in the team. This paragraph is mainly concerned with the publications of last year results.
Publications: [https://hal.inria.fr/hal-01254482], [https://hal.archives-ouvertes.fr/hal-01425021], [https://hal.inria.fr/hal-01287182], [https://hal.inria.fr/hal-01287181], [https://hal.inria.fr/hal-01426666], [16], [27], [30], [28], [31], [21].

6.7. Signal analysis of ultrasonic dental response

Participants: H. Yahia, G. Rosi, S. Jaffard, S. Seuret.
The long-term success of a dental implant is related to the properties of the bone-implant interface. It is important to follow the evolution of bone remodeling phenomena around the implant. Methods based on ultrasound wave propagation were already successfully used by collaborators, in the qualitative and quantitative evaluation of primary and secondary stability of dental implants. Results, numerical and experimental, are analysed with signal processing tools based on multifractal methods. Analysis of the first results shows that these methods are potentially efficient in this case because they can explore and exploit the multi-scale structure of the signal.
Publication: [22].

6.8. Complexity in Electrophysiological Dynamics

Participants: O. Pont, H. Yahia, B. Xu.
Action potentials play an important role in the dynamics of cell-cell communication and they are thus of key relevance in neural tissues. We show that typical real-world electrophysiological signals, with smooth deviations from harmonicity, are typically well described with just the first few terms and result in a rather compact, sparse representation. In particular, we have done an analysis of FitzHugh-Nagumo impulse trains; we have found that 3 anharmonic terms reconstruct better than an equivalent 8-term Fourier representation, with less than half the PSNR and no artifacts from Gibbs phenomenon.
Publication: [17].

6.9. Nonlinear trend removal and heart rate variability analysis

Participants: B. Xu, R. Dubois, O. Pont, H. Yahia.
Publication: [29].

INOCS Team

6. New Results

6.1. Large scale complex structure optimization

New decomposition methods for the time-dependent combined network design and routing problem: A significant amount of work has been focussed on the design of telecommunication networks. The performance of different Integer Programming models for various situations has been computationally assessed. One of the settings that has been thoroughly analyzed is a variant where routing decisions (for time-dependent traffic demand), and network design, are combined in a single optimization model. Solving this model with a state-of-the-art solver on representative network topologies, shows that this model quickly becomes intractable. With an extended formulation, both the number of continuous flow variables and the number of fixed charge capacity constraints are multiplied by a factor $|V|$ (where V represents the set of nodes) leading to large model. However, the linear relaxation of this extended formulation yields much better lower bounds. Nevertheless, even if the extended model provides stronger lower bounds than the aggregated formulation, it suffers from its huge size: solving the linear relaxation of the problem quickly becomes intractable when the network size increases, making the linear relaxation expensive to solve. This observation motivates the analysis of decomposition methods [30].

Convex piecewise linear unsplittable multicommodity flow problems We studied the multi-commodity flow problem with unsplittable flows, and piecewise-linear costs on the arcs. They show that this problem is NP-hard when there is more than one commodity. We propose a new MILP models for this problem, that was compared to two formulations commonly used in the literature. The computational experiments reveal that the new model is able to obtain very strong lower bounds, and is very efficient to solve the considered problem [40].

Tree Reconstruction Problems: We studied the problem of reconstructing a tree network by knowing only its set of terminal nodes and their pairwise distances, so that the reconstructed network has its total edge weight minimized. This problem has applications in several areas, namely the inference of phylogenetic trees and the inference of routing networks topology. Phylogenetic trees allow the understanding of the evolutionary history of species and can assist in the development of vaccines and the study of biodiversity. The knowledge of the routing network topology is the basis for network tomography algorithms and it is a key strategy to the development of more sophisticated and ambitious traffic control protocols and dynamic routing algorithms [31].

Comparison of formulations and solution methods for the discrete ordered p-median problem: We presented several new formulations for the Discrete Ordered Median Problem (DOMP) based on its similarity with some scheduling problems. Some of the new formulations present a considerably smaller number of constraints to define the problem with respect to some previously known formulations. Furthermore, the lower bounds provided by their linear relaxations improve the ones obtained with previous formulations in the literature even when strengthening is not applied. We also present a polyhedral study of the assignment polytope of our tightest formulation showing its proximity to the convex hull of the integer solutions of the problem. Several resolution approaches, among which we mention a branch and cut algorithm, are compared. Extensive computational results on two families of instances, namely randomly generated and from Beasley's OR-library, show the power of our methods for solving DOMP [34].

New models and algorithms for integrated vehicle routing problems

We address a real-life inventory routing problem, which consists in designing routes and managing the inventories of the customers simultaneously. The problem was introduced during the 2016 ROADEF/EURO challenge. The proposed problem is original and complex for several reasons : the logistic ratio optimization objective, the hourly time-granularity for inventory constraints, the driver/trailer allocation management. Clearly, this problem is an optimization problem with complexe structure, for which we proposed a branch-cut-and-price based method : a cut and-column generation procedure was developed, along with a heuristic pricing algorithm to generate new columns and a heuristic fixing procedure to generate integer solutions. The solution method allowed the team including INOCS members to qualify to the final phase of the ROADEF/EURO challenge 2016 [41].

Column generation approach for pure parsimony haplotyping: The knowledge of nucleotides chains that compose the double DNA chain of an individual has a relevant role in detecting diseases and studying populations. However, determining experimentally the single nucleotides chains that, paired, form a certain portion of the DNA is expensive and time-consuming. Mathematical programming approaches have been proposed instead, e.g. formulating the Haplotype Inference by Pure Parsimony problem (HIPP). Abstractly, we are given a set of genotypes (strings over a ternary alphabet 0, 1, 2) and we want to determine the smallest set of haplotypes (binary strings over the set 0, 1) so that each genotype can be 'generated' by some pair of haplotypes, meaning that they are compatible with the genotype and can fully explain its structure. In order to deal with larger instances, we proposed a new model involving an exponential number of variables to be solved via column generation, where variables are dynamically introduced into the model by iteratively solving a pricing problem. We compared different ways of solving the pricing problem, based on integer programming, smart enumeration and local search heuristic. The efficiency of the approach is improved by stabilization and by a heuristic to provide a good initial solution. Results show that, with respect to the linear relaxations of both the polynomial and exponential-size models, our approach yields a tighter formulation and outperforms in both efficiency and effectiveness the previous model for instances with a large number of genotypes [39].

6.2. Bilevel Programming

Bilevel approaches for energy management problems: We have proposed the first bilevel pricing models to explore the relationship between energy suppliers and customers who are connected to a smart grid. Due to their definition, bilevel models enable to integrate customer response into the optimization process of supplier who aims to maximize revenue or minimize capacity requirements. In our setting, the energy provider acts as a leader (upper level) that takes into account a smart grid (lower level) that minimizes the sum of users' disutilities. The latter bases its decisions on the hourly prices set by the leader, as well as the schedule preferences set by the users for each task. The pricing problems, we model, belong to the category of single leader single follower problems. Considering both the monopolistic and competitive environment we present two bilevel bilinear bilinear problems with continuous variables. Heuristics solutions methods are defined to solve large size instances of the models. They are based on the interactions between prices, schedules and peaks. Numerical results on randomly generated instances illustrate numerically the validity of the approach, which achieves an 'optimal trade-off between three objectives: revenue, user cost, and peak demand. Moreover, they put into highlight the ability of the heuristics to produce high quality results compared to the solution of MIP reformulations of the models[36].

New formulations for solving Stackelberg games: We analyzed general Stackelberg games (SGs) and Stackelberg security games (SSGs). SGs are hierarchical adversarial games where players select actions or strategies to optimize their payoffs in a sequential manner. SSGs are a type of SGs that arise in security applications, where the strategies of the player that acts first consist in protecting subsets of targets and the strategies of the followers consist in attacking one of the targets. We review existing mixed integer optimization formulations in both the general and the security setting and present new formulations for the the second one. We compare the SG formulations and the SSG formulations both from a theoretical and a computational point of view. We indentify which formulations provide tighter linear relaxations and show that the strongest formulation for the security version is ideal in the case of one single attacker. Our computational experiments show that the new formulations can be solved in shorter times [46].

6.3. Robust/Stochastic programming

Decomposition method for stochastic staff management problems : We addressed an integrated shift scheduling and load assignment optimization problem for attended home delivery, which is a last-mile delivery service requiring the presence of the customer for the delivery. We were mainly interested in generating a daily master plan for each courier. We proposed a tactical problem integrating a shift scheduling problem and a load assignment problem under demand uncertainty, which was modeled as a two-stage stochastic programming model. This model integrates two types of decisions. First-stage decisions are related to the design of a schedule that includes the periods of the day in which each courier must work and the o-d pairs to visit at each time period. Second-stage decisions (recourse actions) consist of the allocation of a number of packages to be delivered at each time period, for each o-d pair, by each courier, such that the demand (number of packages to deliver) for each scenario is satisfied. Recourse is the ability to take corrective actions after a random event has taken place. The objective is to minimize the sum of the daily staffing cost plus the expected daily recourse cost. To solve this problem, we proposed and implemented a multi-cut integer L-shaped algorithm, where the second stage decomposes by time periods and by demand scenarios. To strengthen the first stage model, some valid inequalities are added, and some of the existing constraints are lifted. Results on real-world based instances from a delivery company demonstrate that our approach provides robust tactical solutions that easily accommodate to fluctuations in customer orders, preventing additional costs related to the underutilization of couriers and the use of external couriers to satisfy all delivery requests [37], [43].

MISTIS Project-Team

7. New Results

7.1. Mixture models

7.1.1. High dimensional Kullback-Leilbler divergence for supervised clustering

Participant: Stephane Girard.

Joint work with: C. Bouveyron (Univ. Paris 5), M. Fauvel and M. Lopes (ENSAT Toulouse))

In the PhD work of Charles Bouveyron [74], we proposed new Gaussian models of high dimensional data for classification purposes. We assume that the data live in several groups located in subspaces of lower dimensions. Two different strategies arise:

- the introduction in the model of a dimension reduction constraint for each group
- the use of parsimonious models obtained by imposing to different groups to share the same values of some parameters

This modelling yielded a supervised classification method called High Dimensional Discriminant Analysis (HDDA) [4]. Some versions of this method have been tested on the supervised classification of objects in images. This approach has been adapted to the unsupervised classification framework, and the related method is named High Dimensional Data Clustering (HDDC) [3]. In the framework of Mailys Lopes PhD, our recent work [50], consists in adapting this work to the classification of grassland management practices using satellite image time series with high spatial resolution. The study area is located in southern France where 52 parcels with three management types were selected. The spectral variability inside the grasslands was taken into account considering that the pixels signal can be modeled by a Gaussian distribution. A parsimonious model is discussed to deal with the high dimension of the data and the small sample size. A high dimensional symmetrized Kullback-Leibler divergence (KLD) is introduced to compute the similarity between each pair of grasslands. The model is positively compared to the conventional KLD to construct a positive definite kernel used in SVM for supervised classification.

7.1.2. Single-run model selection in mixtures

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Russel Steele, McGill University, Montreal, Canada.

A number of criteria exist to select the number of components in a mixture automatically based on penalized likelihood criteria (eg. AIC, BIC, ICL etc.) but they usually require to run several models for different number of components to choose the best one. In this work, the goal was to investigate existing alternatives that can select the component number from a single run and to develop such a procedure for our MRI analysis. These objectives were achieved for the main part as 1) different single run methods have been implemented and tested for Gaussian and Standard mixture models, 2) a Bayesian version of Generalized Student mixtures have been designed that allows the use of the methods in 1), and 3) we also proposed a new heuristic based on this Bayesian model that shows good performance and lower computational times. A more complete validation on simulated data and tests on real MRI data need still to be performed. The single run methods studied are based on a fully Bayesian approach involving therefore specification of appropriate priors and choice of hyperparameters. To estimate our Bayesian mixture model, we use a Variational Expectation-Maximization algorithm (VEM). For the heuristic, we add an additional step inside VEM in order to compute in parallel the corresponding VEM step with one less component. If the lower-bound of the model likelihood is higher with one less component, then we delete this component and go to the next VEM step, until convergence of the algorithm. As regards software development, the Rcpp package has been used to bridge pure R code with more efficient C++ code. This project has been initiated with Alexis Arnaud's visit to McGill University in Montreal in the context of his Mitacs award.

7.1.3. Sequential Quasi Monte Carlo for Dirichlet Process Mixture Models

Participant: Julyan Arbel.

Joint work with: Jean-Bernard Salomond (Université Paris-Est).

In mixture models, latent variables known as allocation variables play an essential role by indicating, at each iteration, to which component of the mixture observations are linked. In sequential algorithms, these latent variables take on the interpretation of particles. We investigate the use of quasi Monte Carlo within sequential Monte Carlo methods (a technique known as sequential quasi Monte Carlo) in nonparametric mixtures for density estimation. We compare them to sequential and non sequential Monte Carlo algorithms. We highlight a critical distinction of the allocation variables exploration of the latent space under each of the three sampling approaches. This work has been presented at the *Practical Bayesian Nonparametrics* NIPS workshop [48].

7.1.4. Truncation error of a superposed gamma process in a decreasing order representation

Participant: Julyan Arbel.

Joint work with: Igor Prünster (University Bocconi, Milan).

Completely random measures (CRM) represent a key ingredient of a wealth of stochastic models, in particular in Bayesian Nonparametrics for defining prior distributions. CRMs can be represented as infinite random series of weighted point masses. A constructive representation due to Ferguson and Klass provides the jumps of the series in decreasing order. This feature is of primary interest when it comes to sampling since it minimizes the truncation error for a fixed truncation level of the series. We quantify the quality of the approximation in two ways. First, we derive a bound in probability for the truncation error. Second, we study a moment-matching criterion which consists in evaluating a measure of discrepancy between actual moments of the CRM and moments based on the simulation output. This work focuses on a general class of CRMs, namely the superposed gamma process, which suitably transformed have already been successfully implemented in Bayesian Nonparametrics. To this end, we show that the moments of this class of processes can be obtained analytically. This work has been presented at the *Advances in Approximate Bayesian Inference* NIPS workshop [47].

7.1.5. Non linear mapping by mixture of regressions with structured covariance matrix

Participant: Emeline Perthame.

Joint work with: Emilie Devijver (KU Leuven, Belgium) and Mélina Gallopin (Université Paris Sud).

In genomics, the relation between phenotypical responses and genes are complex and potentially non linear. Therefore, it could be interesting to provide biologists with statistical models that mimic and approximate these relations. In this paper, we focus on a dataset that relates genes expression to the sensitivity to alcohol of drosophila. In this framework of non linear regression, GLLiM (Gaussian Locally Linear Mapping) is an efficient tool to handle non linear mappings in high dimension. Indeed, this model based on a joint modeling of both responses and covariates by Gaussian mixture of regressions has demonstrated its performance in non linear prediction for multivariate responses when the number of covariates is large. This model also allows the addition of latent factors which have led to interesting interpretation of the latent factors in image analysis. Nevertheless, in genomics, biologists are more interested in graphical models, representing gene regulatory networks. For this reason, we developed an extension of GLLiM in which covariance matrices modeling the dependence structure of genes in each clusters are blocks diagonal, using tools derived for graphical models. This extension provides a new class of interpretable models that are suitable to genomics application fields while keeping interesting prediction properties.

7.1.6. Extended GLLiM model for a subclustering effect: Mixture of Gaussian Locally Linear Mapping (MoGLLiM)

Participant: Florence Forbes.

Joint work with: Naisyin Wang and Chun-Chen Tu from University of Michigan, Ann Arbor, USA.

The work of Chun-Chen Tu and Naisyin Wang pointed out a problem with the original GLLiM model that they propose to solve with a divide-remerge method. The proposal seems to be efficient on test data but the resulting procedure does not anymore correspond to the optimization of a single statistical model. The idea of this work is then to discuss the possibility to change the original GLLiM model in order to account for sub-clusters directly. A small change in the definition seems to have such an effect while remaining tractable. However, we will probably have to be careful with potential non-identifiability issue when dealing with clusters and sub-clusters.

7.2. Semi and non-parametric methods

7.2.1. Robust estimation for extremes

Participants: Clement Albert, Stephane Girard.

Joint work with: M. Stehlik (Johannes Kepler Universitat Linz, Austria and Universidad de Valparaiso, Chile) and A. Dutfoy (EDF R&D).

In the PhD thesis of Clément Albert (funded by EDF), we study the sensitivity of extreme-value methods to small changes in the data [46]. To reduce this sensitivity, robust methods are needed and, in [21], we proposed a novel method of heavy tails estimation based on a transformed score (the t-score). Based on a new score moment method, we derive the t-Hill estimator, which estimates the extreme value index of a distribution function with regularly varying tail. t-Hill estimator is distribution sensitive, thus it differs in e.g. Pareto and log-gamma case. Here, we study both forms of the estimator, i.e. t-Hill and t-lgHill. For both estimators we prove weak consistency in moving average settings as well as the asymptotic normality of t-lgHill estimator in the i.i.d. setting. In cases of contamination with heavier tails than the tail of original sample, t-Hill outperforms several robust tail estimators, especially in small sample situations. A simulation study emphasizes the fact that the level of contamination is playing a crucial role. We illustrate the developed methodology on a small sample data set of stake measurements from Guanaco glacier in Chile. This methodology is adapted to bounded distribution tails in [26] with an application to extreme snow loads in Slovakia.

7.2.2. Conditional extremal events

Participant: Stephane Girard.

Joint work with: L. Gardes (Univ. Strasbourg) and J. Elmethni (Univ. Paris 5)

The goal of the PhD theses of Alexandre Lekina and Jonathan El Methni was to contribute to the development of theoretical and algorithmic models to tackle conditional extreme value analysis, *ie* the situation where some covariate information X is recorded simultaneously with a quantity of interest Y. In such a case, the tail heaviness of Y depends on X, and thus the tail index as well as the extreme quantiles are also functions of the covariate. We combine nonparametric smoothing techniques [77] with extreme-value methods in order to obtain efficient estimators of the conditional tail index and conditional extreme quantiles. When the covariate is functional and random (random design) we focus on kernel methods [18].

Conditional extremes are studied in climatology where one is interested in how climate change over years might affect extreme temperatures or rainfalls. In this case, the covariate is univariate (time). Bivariate examples include the study of extreme rainfalls as a function of the geographical location. The application part of the study is joint work with the LTHE (Laboratoire d'étude des Transferts en Hydrologie et Environnement) located in Grenoble [31], [32].

7.2.3. Estimation of extreme risk measures

Participant: Stephane Girard.

Joint work with: A. Daouia (Univ. Toulouse), L. Gardes (Univ. Strasbourg) and G. Stupfler (Univ. Aix-Marseille).

One of the most popular risk measures is the Value-at-Risk (VaR) introduced in the 1990's. In statistical terms, the VaR at level $\alpha \in (0,1)$ corresponds to the upper α-quantile of the loss distribution. The Value-at-Risk however suffers from several weaknesses. First, it provides us only with a pointwise information: VaR(α) does not take into consideration what the loss will be beyond this quantile. Second, random loss variables with light-tailed distributions or heavy-tailed distributions may have the same Value-at-Risk. Finally, Value-at-Risk is not a coherent risk measure since it is not subadditive in general. A first coherent alternative risk measure is the Conditional Tail Expectation (CTE), also known as Tail-Value-at-Risk, Tail Conditional Expectation or Expected Shortfall in case of a continuous loss distribution. The CTE is defined as the expected loss given that the loss lies above the upper α-quantile of the loss distribution. This risk measure thus takes into account the whole information contained in the upper tail of the distribution. In [64], we investigate the extreme properties of a new risk measure (called the Conditional Tail Moment) which encompasses various risk measures, such as the CTE, as particular cases. We study the situation where some covariate information is available under some general conditions on the distribution tail. We thus has to deal with conditional extremes (see paragraph 7.2.2).

A second possible coherent alternative risk measure is based on expectiles [63]. Compared to quantiles, the family of expectiles is based on squared rather than absolute error loss minimization. The flexibility and virtues of these least squares analogues of quantiles are now well established in actuarial science, econometrics and statistical finance. Both quantiles and expectiles were embedded in the more general class of M-quantiles as the minimizers of a generic asymmetric convex loss function. It has been proved very recently that the only M-quantiles that are coherent risk measures are the expectiles.

7.2.4. Multivariate extremal events

Participants: Stephane Girard, Florence Forbes.

Joint work with: F. Durante (Univ. Bolzen-Bolzano, Italy) and G. Mazo (Univ. Catholique de Louvain, Belgique).

Copulas are a useful tool to model multivariate distributions [83]. However, while there exist various families of bivariate copulas, much fewer has been done when the dimension is higher. To this aim an interesting class of copulas based on products of transformed copulas has been proposed in the literature. The use of this class for practical high dimensional problems remains challenging. Constraints on the parameters and the product form render inference, and in particular the likelihood computation, difficult. As an alternative, we proposed a new class of copulas constructed by introducing a latent factor. Conditional independence with respect to this factor and the use of a nonparametric class of bivariate copulas lead to interesting properties like explicitness, flexibility and parsimony. In particular, various tail behaviours are exhibited, making possible the modeling of various extreme situations [17], [22].

7.2.5. Level sets estimation

Participant: Stephane Girard.

Joint work with: G. Stupfler (Univ. Aix-Marseille).

The boundary bounding the set of points is viewed as the larger level set of the points distribution. This is then an extreme quantile curve estimation problem. We proposed estimators based on projection as well as on kernel regression methods applied on the extreme values set, for particular set of points [10]. We also investigate the asymptotic properties of existing estimators when used in extreme situations. For instance, we have established in collaboration with G. Stupfler that the so-called geometric quantiles have very counter-intuitive properties in such situations [20] and thus should not be used to detect outliers.

7.2.6. Robust Sliced Inverse Regression.

Participants: Stephane Girard, Alessandro Chiancone, Florence Forbes.

This research theme was supported by a LabEx PERSYVAL-Lab project-team grant.

Sliced Inverse Regression (SIR) has been extensively used to reduce the dimension of the predictor space before performing regression. Recently it has been shown that this technique is, not surprisingly, sensitive to noise. Different approaches have thus been proposed to robustify SIR. In [14], we start considering an inverse problem proposed by R.D. Cook and we show that the framework can be extended to take into account a non-Gaussian noise. Generalized Student distributions are considered and all parameters are estimated via an EM algorithm. The algorithm is outlined and tested comparing the results with different approaches on simulated data. Results on a real dataset show the interest of this technique in presence of outliers.

7.2.7. Collaborative Sliced Inverse Regression.

Participants: Stephane Girard, Alessandro Chiancone.

This research theme was supported by a LabEx PERSYVAL-Lab project-team grant.

Joint work with: J. Chanussot (Gipsa-lab and Grenoble-INP).

In his PhD thesis work, Alessandro Chiancone studies the extension of the SIR method to different sub-populations. The idea is to assume that the dimension reduction subspace may not be the same for different clusters of the data [15]. One of the difficulty is that standard Sliced Inverse Regression (SIR) has requirements on the distribution of the predictors that are hard to check since they depend on unobserved variables. It has been shown that, if the distribution of the predictors is elliptical, then these requirements are satisfied. In case of mixture models, the ellipticity is violated and in addition there is no assurance of a single underlying regression model among the different components. Our approach clusterizes the predictors space to force the condition to hold on each cluster and includes a merging technique to look for different underlying models in the data. A study on simulated data as well as two real applications are provided. It appears that SIR, unsurprisingly, is not able to deal with a mixture of Gaussians involving different underlying models whereas our approach is able to correctly investigate the mixture.

7.2.8. Hapke's model parameter estimation from photometric measurements

Participants: Florence Forbes, Emeline Perthame.

Joint work with: Sylvain Douté (IPAG, Grenoble).

The Hapke's model is a widely used analytical model in planetology to describe the spectro-photometry of granular materials. It is a non linear model F that links a set of parameters x to a "theoretical" Bidirectional Reflectance Diffusion Function (BRDF). In practice, we assume that the observed BRDF Y is a noisy version of the "theoretical" one

$$Y = F(x) + \epsilon \tag{12}$$

where ϵ is a centered Gaussian noise with diagonal covariance matrix Σ. Then x is also assumed to be random with some prior distribution to be specified, e.g. uniform on the parameters range in [84]. The overall goal is to estimate the posterior distribution $p(x|y)$ for some observed BRDF y. Equation (5) defines the likelihood of the model which is $p(y|x) = \mathcal{N}(y; F(x), \Sigma)$. Then since F is non linear, it is not possible to obtain an analytical expression for $p(x|y)$. However, it is easy to simulate parameters x that follows the posterior distribution $p(x|y) \propto p(y|x)\ p(x)$ for instance using MCMC techniques [84]. If only point estimate are desired, the MAP can be used and evolutionary algorithms can then be used also using $p(y|x)\ p(x)$ as a fitness function. But obtaining such simulations is time consuming and has to be done for each observed value of y. In this work, we propose to use a locally linear mapping approximation and an inverse regression strategy to provide an analytical expression of $p(x|y)$. The idea is that the non linear F can be approximated by a number K of locally linear functions and that each of this function is easy to inverse. It follows that the inverse of F is also approximated as locally linear. Preliminary results were presented at the MultiPlaNet workshop in Orsay, December 14, 2016. They show that the proposed method does not fully reproduce the previous results obtained using MCMC techniques. Further investigations are required to understand the origin of the difference. Also ABC (approximate Bayes computation) methods will be considered as a subsequent step that may improved the current procedure while remaining computationally efficient.

7.2.9. Prediction intervals for inverse regression models in high dimension

Participant: Emeline Perthame.

Joint work with: Emilie Devijver (KU Leuven, Belgium).

Inverse regression, as a dimension reduction technique, is a reliable and efficient approach to handle large regression issues in high dimension, when the number of features exceeds the number of observations. Indeed, under some conditions, dealing with the inverse regression problem associated to a forward regression problem drastically reduces the number of parameters to estimate and make the problem tractable. However, regression models are often used to predict a new response from a new observed profile of covariates, and we may be interested in deriving confidence bands for the prediction to quantify the uncertainty around a predicted response. Theoretical results have already been derived for the well-known linear model, but recently, the curse of dimensionality has increased the interest of practitioners and theoreticians into generalization of those results on a high-dimension context. When both the responses and the covariates are multivariate, we derive in this work theoretical prediction bands for the inverse regression linear model and propose an analytical expression of these intervals. The feasibility, the confidence level and the accuracy of the proposed intervals are also analyzed through a simulation study.

7.2.10. Multi sensor fusion for acoustic surveillance and monitoring

Participants: Florence Forbes, Jean-Michel Becu.

Joint work with: Pascal Vouagner and Christophe Thirard from ACOEM company.

In the context of the DGA-rapid WIFUZ project with the ACOEM company, we addressed the issue of determining the localization of shots from multiple measurements coming from multiple sensors. We used Bayesian inversion and simulation techniques to recover multiple sources mimicking collaborative interaction between several vehicles. This project is at the intersection of data fusion, statistics, machine learning and acoustic signal processing. The general context is the surveillance and monitoring of a zone acoustic state from data acquired at a continuous rate by a set of sensors that are potentially mobile and of different nature. The overall objective is to develop a prototype for surveillance and monitoring that is able to combine multi sensor data coming from acoustic sensors (microphones and antennas) and optical sensors (infrared cameras) and to distribute the processing to multiple algorithmic blocs.

7.3. Graphical and Markov models

7.3.1. Conditional independence properties in compound multinomial distributions

Participant: Jean-Baptiste Durand.

Joint work with: Pierre Fernique (Inria, Virtual Plants) and Jean Peyhardi (Université de Montpellier).

We developed a unifying view of two families of multinomial distributions: the singular – for modeling univariate categorical data – and the non-singular – for modeling multivariate count data. In the latter model, we introduced sum-compound multinomial distributions that encompass re-parameterization of non-singular multinomial and negative multinomial distributions. The estimation properties within these compound distributions were obtained, thus generalizing know results in univariate distributions to the multivariate case. These distributions were used to address the inference of discrete-state models for tree-structured data. In particular, they were used to introduce parametric generation distributions in Markov-tree models [66].

7.3.2. Change-point models for tree-structured data

Participant: Jean-Baptiste Durand.

Joint work with: Pierre Fernique (Inria) and Yann Guédon (CIRAD), Inria Virtual Plants.

In the context of plant growth modelling, methods to identify subtrees of a tree or forest with similar attributes have been developed. They rely either on hidden Markov modelling or multiple change-point approaches. The latter are well-developed in the context of sequence analysis, but their extensions to tree-structured data are not straightforward. Their advantage on hidden Markov models is to relax the strong constraints regarding dependencies induced by parametric distributions and local parent-children dependencies. Heuristic approaches for change-point detection in trees were proposed and applied to the analysis of patchiness patterns (consisting of canopies made of clumps of either vegetative or flowering botanical units) in mango trees [43].

7.3.3. Hidden Markov models for the analysis of eye movements

Participants: Jean-Baptiste Durand, Brice Olivier.

This research theme is supported by a LabEx PERSYVAL-Lab project-team grant.

Joint work with: Marianne Clausel (LJK) Anne Guérin-Dugué (GIPSA-lab) and Benoit Lemaire (Laboratoire de Psychologie et Neurocognition)

In the last years, GIPSA-lab has developed computational models of information search in web-like materials, using data from both eye-tracking and electroencephalograms (EEGs). These data were obtained from experiments, in which subjects had to make some kinds of press reviews. In such tasks, reading process and decision making are closely related. Statistical analysis of such data aims at deciphering underlying dependency structures in these processes. Hidden Markov models (HMMs) have been used on eye movement series to infer phases in the reading process that can be interpreted as steps in the cognitive processes leading to decision. In HMMs, each phase is associated with a state of the Markov chain. The states are observed indirectly though eye-movements. Our approach was inspired by Simola et al. (2008), but we used hidden semi-Markov models for better characterization of phase length distributions. The estimated HMM highlighted contrasted reading strategies (ie, state transitions), with both individual and document-related variability. However, the characteristics of eye movements within each phase tended to be poorly discriminated. As a result, high uncertainty in the phase changes arose, and it could be difficult to relate phases to known patterns in EEGs.

This is why, as part of Brice Olivier's PhD thesis, we are developing integrated models coupling EEG and eye movements within one single HMM for better identification of the phases. Here, the coupling should incorporate some delay between the transitions in both (EEG and eye-movement) chains, since EEG patterns associated to cognitive processes occur lately with respect to eye-movement phases. Moreover, EEGs and scanpaths were recorded with different time resolutions, so that some resampling scheme must be added into the model, for the sake of synchronizing both processes.

To begin with, we first proved why HMM would be the best option in order to conduct this analysis and what could be the alternatives. A brief state of the art was made on models similar to HMMs. However, since our data is very specific, we needed to make use of unsupervised graphical generative models for the analysis of sequences which would keep a deep meaning. It resulted that Hidden semi-Markov model (HSMM) was the most powerful tool satisfying all our needs. Indeed, a HSMM is characterized by meaningful parameters such as an initial distribution, transition distributions, emission distributions and sojourn distributions, which allows us to directly characterize a reading strategy. Second, we found and improved an existing implementation of such a model. After searching for libraries to make inference in HSMM, the Vplants library embedded in the OpenAlea software turned out to be the most viable solution regarding the functionalities, though it was still incomplete. Consequently, we proposed improvements to this library and added functions in order to boost the likelihood of the data. This lead us to also propose a new library included in that software which is specific at the analysis of eye movements. Third, in order to improve and validate the interpretation of the reading strategies, we calculated indicators specific to each reading strategy. Fourth, since the parameters obtained from the model suggested individual and text variability, we first investigated text clustering to reduce the variability of the model. In order to do this, we supervised a group of 6 students to explore the text clustering component with the mission of clustering the texts by evolution of the semantic similarity throughout text. We therefore explored different methods for time series clustering and we retained the usage of Ascendant Hierarchical Clustering (AHC) using the Dynamic Time Warping (DTW) metric, which allows global dynamics of the time series to be captured, but not local dynamics. Plus, we preferred the simplicity and good understanding of the results using that method. Therefore, we deduced three text profiles giving meaning to the evolution of the semantic similarity: a step profile, a ramp profile, and a saw profile. With that new information in hand, we are now able to decompose our model over text profiles and hence, reduce its variability.

As discussed in the previous section, our work is focused on the standalone analysis of the eye-movements. We are currently polishing this phase of work. The common work and the goal for this coming year is to develop and implement a model for jointly analyzing eye-movements and EEGs in order to improve the discrimination of the reading strategies.

7.3.4. Lossy compression of tree structures

Participant: Jean-Baptiste Durand.

Joint work with: Christophe Godin (Inria, Virtual Plants) and Romain Azais (Inria BIGS)

In a previous work [79], a method to compress tree structures and to quantify their degree of self-nestedness was developed. This method is based on the detection of isomorphic subtrees in a given tree and on the construction of a DAG (Directed Acyclic Graph), equivalent to the original tree, where a given subtree class is represented only once (compression is based on the suppression of structural redundancies in the original tree). In the lossless compressed graph, every node representing a particular subtree in the original tree has exactly the same height as its corresponding node in the original tree. A lossy version of the algorithm consists in coding the nearest self-nested tree embedded in the initial tree. Indeed, finding the nearest self-nested tree of a structure without more assumptions is conjectured to be an NP-complete or NP-hard problem. We obtained new theoretical results on the combinatorics of self-nested structures [60]. We improved this lossy compression method by computing a self-nested reduction of a tree that better approximates the initial tree. The algorithm has polynomial time complexity for trees with bounded outdegree. This approximation relies on an indel edit distance that allows (recursive) insertion and deletion of leaf vertices only. We showed using a simulated dataset that the error rate of this lossy compression method is always better than the loss based on the nearest embedded self-nestedness tree [79] while the compression rates are equivalent. This procedure is also a keystone in our new topological clustering algorithm for trees. Perspectives of improving the time complexity of our algorithm include taking profit from one of its byproduct, which could be used as an indicator of both the number of potential candidates to explore and of the proximity of the tree to the nearest self-nested tree.

7.3.5. Learning the inherent probabilistic graphical structure of metadata

Participants: Thibaud Rahier, Stephane Girard, Florence Forbes.

Joint work with: Sylvain Marié, Schneider Electric.

The quality of prediction and inference on temporal data can be significantly improved by taking advantage of the associated metadata. However, metadata are often only partially structured and may contain missing values. In the context of T. Rahier's PhD with Schneider Electric, we first considered the problem of learning the inherent probabilistic graphical structure of metadata, which has two main benefits: (i) graphical models are very flexible and therefore enable the fusion of different types of data together (ii) the learned graphical model can be interrogated to perform tasks on metadata alone: variable clustering, conditional independence discovery or missing data replenishment. Bayesian Network (and more generally Probabilistic Graphical Model) structure learning is a tremendous mathematical challenge, that involves a NP-Hard optimisation problem. In the past year, we have explored many approaches to tackle this issue, and begun to develop a tailor-made algorithm, that exploits dependencies typically present in metadata, and that significantly speeds up the structure learning task and increases the chance of finding the optimal structure.

7.3.6. Robust Graph estimation

Participants: Karina Ashurbekova, Florence Forbes.

Joint work with: Sophie Achard, CNRS, Gipsa-lab.

In the face of increasingly high dimensional data and of trying to understand the dependency/association present in the data the literature on graphical modelling is growing rapidly and covers a range of applications (from bioinformatics e.g gene expression data to document modelling). A major limitation of recent work on using the (standard) Student t distribution for robust graphical modelling is the lack of independence and conditional independence of the Student t distribution, and estimation in this context (with the standard student t) is very difficult. We propose to develop and assess a generalized Student t from a new family (which has independence and conditional independence as special properties) for the general purpose of graphical modelling in high dimensional settings. Its main characteristic is to include multivariate heavy-tailed distributions with variable marginal amounts of tailweight that allow more complex dependencies than the standard case. We target an application to brain connectivity data for which standard Gaussian graphical models have been applied. Brain connectivity analysis consists in the study of multivariate time series representing local dynamics at each of multiple sites or sources throughout the whole human brain while functioning using for example functional magnetic resonance imaging (fMRI). The acquisition is difficult and often spikes are observed due to the movement of the subjects inside the scanner. In the case of identifying Gaussian graphical models, the glasso technique has been developed for estimating sparse graphs. However, this method can be severely impacted by the inclusion of only a few contaminated values, such as spikes that commonly occur in fMRI time series, and the resulting graph has the potential to contain false positive edges. Therefore, our goal was to assess the performance of more robust methods on such data.

7.4. Robust non Gaussian models

7.4.1. Robust Locally linear mapping with mixtures of Student distributions

Participants: Florence Forbes, Emeline Perthame, Brice Olivier.

The standard GLLiM model [6] for high dimensional regression assumes Gaussian noise models and is in its unconstrained version equivalent to a joint GMM. The fact that response and independent variables (X, Y) are jointly a mixture of Gaussian distribution is the key for all derivations in the model. In this work, we show that similar developments are possible based on a joint Student Mixture model, joint SMM. It follows a new model referred to as SLLiM for Student Locally linear mapping for which we investigate the robustness to outlying data in a high dimensional regression context [71]. The corresponding code is available on the CRAN in the *xLLiM* package.

7.4.2. Rectified binaural ratio: A complex T-distributed feature for robust sound localization

Participant: Florence Forbes.

Joint work with: Antoine Deleforge, Inria PANAMA team in Rennes.

Most existing methods in binaural sound source localization rely on some kind of aggregation of phase-and level-difference cues in the time-frequency plane. While different aggregation schemes exist, they are often heuristic and suffer in adverse noise conditions. In this work, we introduce the rectified binaural ratio as a new feature for sound source localization. We show that for Gaussian-process point source signals corrupted by stationary Gaussian noise, this ratio follows a complex t-distribution with explicit parameters. This new formulation provides a principled and statistically sound way to aggregate binaural features in the presence of noise. We subsequently derive two simple and efficient methods for robust relative transfer function and time-delay estimation. Experiments on heavily corrupted simulated and speech signals demonstrate the robustness of the proposed scheme. This work has been presented at the Eusipco conference in 2016 [30].

7.4.3. Statistical reconstruction methods for multi-energy tomography

Participants: Florence Forbes, Pierre-Antoine Rodesch.

Joint work with: Veronique Rebuffel from CEA Grenoble.

In the context of Pierre-Antoine Rodesh's PhD thesis, we investigate new statistical and optimization methods for tomographic reconstruction from non standard detectors providing multiple energy signals.

7.5. Statistical models for Neuroscience

7.5.1. Advanced statistical analysis of functional Arterial Spin Labelling data

Participants: Florence Forbes, Aina Frau Pascual.

Joint work with: Philippe Ciuciu from Team PARIETAL and Neurospin, CEA Saclay.

Arterial Spin Labelling (ASL) is a non-invasive perfusion MR imaging technique that can be also used to measure brain function (fASL for functional ASL). In contrast to BOLD fMRI, it gives a quantitative and absolute measure of cerebral blood flow (CBF), making this modality appealing for clinical neuroscience and patient's follow-up over longitudinal studies. However, its limited signal-to-noise ratio makes the analysis of fASL data challenging. In this work, we compared different approaches (GLM vs JDE) in the analysis of functional ASL data for the detection of evoked brain activity at the group level during visual and motor task performance. Our dataset has been collected at Neurospin on a 3T Tim Trio Siemens scanner (CEA Saclay, France), during the HEROES project (Inria Grant). It contains BOLD data (165 scans, TR=2.5s, TE=30ms, 3x3x3mm3) and functional pulsed ASL data (Q2TIPS PICORE scheme [Luh,00], 165 scans, TR=2.5s, TE=11ms, 3x3x7.5 mm3) of 13 right-handed subjects (7 men and 6 women) of age between 20 and 29. The experimental design consists of a mini-block paradigm of visual, motor and auditory tasks with 16 blocks of 15s each followed by 10s of rest. Data have been scaled, realigned, and normalized. For univariate analysis, the images have also been spatially smoothed with a Gaussian kernel of 5 mm full width half at maximum. Three data analysis approaches have been compared: (a) univariate General Linear Model (GLM) that considers canonical shapes for the perfusion and hemodynamic responses; (b) physiologically informed joint detection estimation (PI-JDE) [4] that jointly estimates effect maps and response functions in a multivariate manner in a Bayesian framework; (c) A restricted version of PI-JDE that considers fixed canonical shapes for the perfusion and hemodynamic responses (PRF and HRF, respectively), defining an intermediate approach between the first two. Since methods (b)-(c) embed adaptive spatial regularization, they do not require a preliminary smoothing of the data. Our results demonstrate that the PI-JDE multivariate approach is a competing alternative to GLM for the analysis of fASL: it recovers more localized and stronger effects. Our findings also replicate the state-of-the-art by showing more localized activation patterns in perfusion as compared to hemodynamics.

7.5.2. BOLD VEM multi session extension of the JDE approach

Participants: Florence Forbes, Aina Frau Pascual.

Joint work with: Philippe Ciuciu from Team PARIETAL and Neurospin, CEA Saclay.

The fast solution of the JDE approach for BOLD fMRI presented in [5] uses a variational expectation maximization (VEM) algorithm and considers a single session of BOLD data. This paper shows the faster performance of this algorithm with respect to the Markov Chain Monte Carlo (MCMC) approach presented in earlier work, with similar results. In fMRI, usually several sessions are acquired for the same subject to be able to compare them or combine them. In [73], a multiple-session extension of the JDE approach has been proposed to analyze several sessions together. The solution proposed uses MCMC and considers that the response levels have a mean value per condition and a common variance between sessions. In the context of Aina Frau's PhD, a VEM solution of this extension has been implemented. Experimental results have shown that the solution of the multiple-session VEM is not very different from the average of the results computed with single session VEM. For this reason, we proposed a heteroscedastic version of the multiple-session VEM. It amounts to considering session-specific variances. The goal is to be able to weight the importance of the different sessions so as to diminish the contribution of any potential noisy session to the final parameter estimates.

7.5.3. Estimating biophysical parameters from multimodal fMRI data

Participants: Florence Forbes, Pablo Mesejo Santiago.

Joint work with: Jan Warnking from Grenoble Institute of Neuroscience.

Functional Magnetic Resonance Imaging (fMRI) indirectly studies brain function. With Jan M. Warnking (Grenoble Institute of Neurosciences) we worked on the estimation of biophysical parameters from fMRI signals. We first used only BOLD signals, using a stochastic population-based optimization method to estimate 15 parameters without neither providing initial estimates nor computing gradients. Initial results were published at MICCAI 2015 and in the IEEE JSTSP journal [81], [82]. Also a MATLAB toolbox was released (see software section). The current ongoing work is to study the impact of the combination of different fMRI modalities in the estimation of this biophysical parameters. We can use 3 fMRI modalities (BOLD, ASL and MION) and 13 rats. We ran our optimizer with all possible combinations of modalities. The initial hypothesis was that as long as we introduce more fMRI modalities we would like to see more consistent estimates but we need to assess possible limits due to potential lack of data: only 13 rats, 6 of them without MION, and potential outliers among the rats that would better be excluded from the analysis.

7.5.4. Multi-subject joint parcelation detection estimation in functional MRI

Participant: Florence Forbes.

Joint work with: Lotfi Chaari, Mohanad Albughdadi, Jean-Yves Tourneret from IRIT-ENSEEIHT in Toulouse and Philippe Ciuciu from Neurospin, CEA Saclay.

fMRI experiments are usually conducted over a population of interest for investigating brain activity across different regions, stimuli and subjects. Multi-subject analysis usually proceeds in two steps: an intra-subject analysis is performed sequentially on each individual and then a group-level analysis is carried out to report significant results at the population level. This work considers an existing Joint Parcellation Detection Estimation (JPDE) model which performs joint hemodynamic parcellation, brain dynamics estimation and evoked activity detection. The hierarchy of the JPDE model is extended for multi-subject analysis in order to perform group-level parcellation. Then, the corresponding underlying dynamics is estimated in each parcel while the detection and estimation steps are iterated over each individual. Validation on synthetic and real fMRI data shows its robustness in inferring group-level parcellation and the corresponding hemodynamic profiles. This work has been presented at ISBI 2016 [42].

7.5.5. Automatic segmentation and characterization of brain tumors using robust multivariate clustering of multiparametric MRI

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Emmanuel Barbier and Benjamin Lemasson from Grenoble Institute of Neuroscience.

Brain tumor segmentation is a difficult task in the field of multiparametric MRI analysis because of the number of maps that are available. Furthermore, the characterization of brain tumors can be time-consuming, even for medical experts, and the reference method is biopsy which is a local and invasive technique. Because of this, it is important to develop automatic and non-invasive approaches in order to help the medical expert with these issues. In this study we use a robust statistical model-based method to classify multiparametric MRI of rat brains. The voxels are gather into classes resulting from multivariate multi-scaled Student distributions, which can accommodate outliers. First we adjust a mixture model on a reference group of rats to learn the MRI characteristics of healthy tissues. Second we use this model to delineate the brain tumors as atypical voxels in the data set of unhealthy rats. Third we adjust a new mixture model only on the atypical voxels to learn the MRI characteristics of tumorous tissues. Finally, we extract a fingerprint for each tumor type to make a tumor dictionary.

Our data set is composed of healthy rats (n=8 rats) and 4 groups of rats bearing a brain tumor model (n=8 per group). For each rat, we acquired 5 quantitative MRI parameters along 5 slices. And the proposed tumor dictionary reaches a rate of 75% of accurate prediction with a leave-one-out procedure.

7.5.6. Monitoring brain tumor evolution using multiparametric MRI

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Emmanuel Barbier, Nora Collomb and Benjamin Lemasson from Grenoble Institute of Neuroscience.

Analyzing brain tumor tissue composition can improve the handling of tumor growth and resistance to therapies. We showed on a 6 time point dataset of 8 rats that multiparametric MRI could be exploited via statistical clustering to quantify intra-lesional heterogeneity in space and time. More specifically, MRI can be used to map structural, eg diffusion, as well as functional, eg volume (BVf), vessel size (VSI), oxygen saturation of the tissue (StO2), characteristics. In previous work, these parameters were analyzed to show the great potential of multiparametric MRI (mpMRI) to monitor combined radio- and chemo-therapies. However, to exploit all the information contained in mpMRI while preserving information about tumor heterogeneity, new methods need to be developed. We demonstrated the ability of clustering analysis applied to longitudinal mpMRI to summarize and quantify intra-lesional heterogeneity during tumor growth. This study showed the interest of a clustering analysis on mpMRI data to monitor the evolution of brain tumor heterogeneity. It highlighted the type of tissue that mostly contributes to tumor development and could be used to refine the evaluation of therapies and to improve tumor prognosis.

7.5.7. Assessment of tissue injury in severe brain trauma

Participant: Florence Forbes.

Joint work with: Michel Dojat and Christophe Maggia from Grenoble Institute of Neuroscience and Senan Doyle from Pixyl.

Traumatic brain injury (TBI) remains a leading cause of death and disability among young people worldwide and current methods to predict long-term outcome are not strong. TBI initiates a cascade of events that can lead to secondary brain damage or exacerbate the primary injury, and these develop hours to days after the initial accident. The concept of secondary brain damage is the focus of modern TBI management in Intensive Care Units. The imbalance between oxygen supply to the brain tissue and utilization, i.e. brain tissue hypoxia, is considered the major cause for the development of secondary brain damage, and hence poor neurological outcome. Monitoring brain tissue oxygenation after TBI using brain tissue O_2 pressure (PbtO_2) probes surgically inserted into the parenchyma, may help clinicians to initiate adequate actions when episodes of brain ischemia/hypoxia are identified. The aggressive treatment of low PbtO_2 values ($<$ 15mmHg for more than 30 minutes) was associated with better outcome compared to standard therapy in some cohort studies of severe head-injury patients. However, another study was unable to find similar benefits to patient outcome. MRI is an excellent modality for estimating global and regional alterations in TBI and for following their longitudinal evolution. To assess the complexity of TBI, several morphological sequences are required for assessing volume loss. Moreover, diffusion tensor imaging (DTI) offers the most sensitive modality for the detection of changes in the acute phase of TBI and increases the accuracy of long-term outcome prediction compared to the available clinical/radiographic prognostic score. Mean Diffusivity (MD) or Apparent Diffusion Coefficient (ADC) have been widely used to determine the volume of ischemic tissue, and assess intra- and extracellular conditions. A reduction of MD is related to cytotoxic edema (intracellular) while an increase of MD indicates a vasogenic edema (extracellular). Changes of MD are expected with severe TBI. The volume of lesions on DTI shows a strong correlation with neurological outcome at patient discharge. We consider a clinically relevant criterion to be the volume of vulnerable brain lesions after TBI, as previously suggested. In consequence, we need an automatic segmentation method to assess the tissue damage in severe trauma, acute phase i.e. before 10 days after the event. Skull deformation, the presence of blood in the acute phase, the high variability of brain damage that excludes the use of anatomical *a priori* information, and the diffuse aspect of brain injury affecting potentially all brain structures, render TBI segmentation particularly demanding. The methods proposed in the literature are mainly concerned with volumetric changes following TBI and scarcely report lesion load. In this work, we report our methodological developments to assess lesion load in severe brain trauma in the entire brain. We use P-LOCUS to perform brain tissue segmentation and exclude voxels labeled as CSF, ventricle and hemorrhagic lesion. We propose a fusion of several atlases to parcel cortical, subcortical and WM structures into well identified regions where MD values can be expected to be homogenous. Abnormal voxels are detected in these regions by comparing MD values with normative values computed from healthy volunteers. The preliminary results, evaluated in a single center, are a first step in defining a robust methodology intended to be used in multi-center studies. This work has been published in [58].

7.5.8. Automatic multiple sclerosis lesion segmentation with P-Locus

Participant: Florence Forbes.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience and Senan Doyle from Pixyl.

P-LOCUS provides automatic quantitative neuroimaging biomarker extraction tools to aid diagnosis, prognosis and follow-up in multiple sclerosis studies. The software performs accurate and precise segmentation of multiple sclerosis lesions in a multi-stage process. In the first step, a weighted Gaussian tissue model is used to perform a robust segmentation. The algorithm avails of complementary information from multiple MR sequences, and includes additional estimated weight variables to account for the relative importance of each voxel. These estimated weights are used to define candidate lesion voxels that are not well described by a normal tissue model. In the second step, the candidate lesion regions are used to populate the weighted Gaussian model and guide convergence to an optimal solution. The segmentation is unsupervised, removing the need for a training dataset, and providing independence from specific scanner type and MRI scanner protocol. The procedure was applied to participate to the MSSEG Challenge at Miccai 2016 in Athen: Multiple Sclerosis Lesions Segmentation Challenge Using a Data Management and Processing Infrastructure [55].

MODAL Project-Team

7. New Results

7.1. An oracle inequality for Quasi-Bayesian Non-Negative Matrix Factorisation

Participant: Benjamin Guedj.

We have extended the quasi-Bayesian perspective to the popular setting of non-negative matrix factorisation. This is a pivotal problem in machine learning (image segmentation, recommendation systems, audio source separation, ...) and we were able to propose an original estimator of the unobserved matrix. An oracle inequality is derived, along with several possible implementations. This work is now submitted to an international journal [38].

Joint work with Pierre Alquier.

7.2. PAC-Bayesian Online Clustering

Participants: Benjamin Guedj, Le Li.

We have extended the PAC-Bayesian framework to online learning. Our algorithm (called PACBO) performs online clustering of random sequences, and is supported by strong theoretical (regret bounds) and algorithmic (ergodicity of an MCMC implementation) results. This work is now submitted to an international journal [46].

Joint work with Sébastien Loustau.

7.3. Simpler PAC-Bayesian Bounds for Hostile Data

Participant: Benjamin Guedj.

We have introduced an original and much simpler way of deriving PAC-Bayesian bounds, through the use of f-divergences (therefore generalizing earlier works on Renyi's divergence and Kullback-Leibler divergence). This work is now submitted to an international conference [39].

Joint work with Pierre Alquier.

7.4. Clustering categorical functional data: Application to medical discharge letters

Participants: Cristian Preda, Cristina Preda, Vincent Vandewalle.

Categorical functional data represented by paths of a stochastic jump process are considered for clustering. For paths of the same length, the extension of the multiple correspondence analysis allows the use of well-known methods for clustering finite dimensional data. When the paths are of different lengths, the analysis is more complex. In this case, for Markov models we have proposed an EM algorithm to estimate a mixture of Markov processes. This work has been presented in a workshop [48].

7.5. Simultaneous dimension reduction and multi-objective clustering

Participant: Vincent Vandewalle.

In model based clustering of quantitative data it is often supposed that only one clustering variable explains the heterogeneity of all the others variables. However, when variables come from different sources, it is often unrealistic to suppose that the heterogeneity of the data can only be explained by one variable. If such an assumption is made, this could lead to a high number of clusters which could be difficult to interpret. A model based multi-objective clustering is proposed, it assumes the existence of several latent clustering variables, each one explaining the heterogeneity of the data on some clustering projection. In order to estimate the parameters of the model an EM algorithm is proposed, it mainly relies on a reinterpretation of the standard factorial discriminant analysis in a probabilistic way. The obtained results are projections of the data on some principal clustering components allowing some synthetic interpretation of the principal clusters raised by the data. This work has been presented in a conference [49].

7.6. Spatial Prediction of solar energy

Participant: Sophie Dabo.

Sophie Dabo-Niang's new result concern a work on spatial prediction of solar Energy in collaboration with some physicians and is now published [15].

This paper introduces a new approach for the forecasting of solar radiation series at a located station for very short time scale. We built a multivariate model in using few stations (3 stations). The proposed model is a spatio temporal vector autoregressive VAR model specifically designed for the analysis of spatially sparse spatio-temporal data. This model differs from classic linear models in using spatial and temporal parameters where the available predictors are the lagged values at each station. A spatial structure of stations is defined by the sequential introduction of predictors in the model. Moreover, an iterative strategy in the process of our model will select the necessary stations removing the uninteresting predictors and also selecting the optimal p-order. We studied the performance of this model. The metric error, the relative root mean squared error (rRMSE), is presented at different short time scales. Moreover, we compared the results of our model to simple and well known persistence model and those found in literature.

7.7. Multiple change-point detection

Participants: Alain Celisse, Guillemette Marot.

This is a joint work with Morgane Pierre-Jean and Guillem Rigaill (Univ. Evry).

The paper related to the work described in previous MODAL team reports (sections Kernel change point) has been pursuied and made available on Arxiv [42]. For recall, this work focuses on the problem of detecting abrupt changes arising in the full distribution of the observations (not only in the mean or variance). It provides greatly improved algorithms in terms of computational complexity (both in time and space). The computational and statistical performances of these new algorithms have been assessed through empirical experiments, which are detailed in the preprint.

7.8. Differential gene expression analysis

Participants: Alain Celisse, Guillemette Marot.

The use of empirical Bayesian techniques implemented in the R package metaMA has enabled to better understand Waldenstrom's macroglobulinemia. The new findings in Biology have been published in [18].

7.9. New concentration inequalities for the leave-p-out CV estimator

Participant: Alain Celisse.

New concentration inequalities have been established for the leave-p-out cross-validation estimator applied to assess the performance the k-nearest neighbour binary classifier. Joint work with Tristan Mary-Huard.

7.10. A new notion of stability for learning algorithms

Participants: Alain Celisse, Benjamin Guedj.

We introduced a new notion of stability for learning algorithms, which bridges the gap between the earlier uniform and hypothesis stability notions. It allows us to derive new PAC exponential concentration inequalities that apply to the Ridge regression algorithm as a first step. The first version of this work is presented in the preprint [41] and is now an active line of research.

7.11. Model for conditionally correlated categorical data

Participants: Christophe Biernacki, Matthieu Marbac Lourdelle, Vincent Vandewalle.

It is a model-based clustering proposal (called CMM for Conditional Modes Model) where categorical data are grouped into conditionally independent blocks. The corresponding block distribution is a parsimonious multinomial distribution where the few free parameters correspond to the most likely modality crossings, while the remaining probability mass is uniformly spread over the other modality crossings. The exact computation of the integrated complete-data likelihood allows to perform the model selection, by a Gibbs sampler, reducing the computing time consuming by parameter estimation and avoiding BIC criterion biases pointed out by our experiments. This work is now published in the international journal Advances in Data Analysis and Classification (Marbac et al, 2016). Furthermore, an R package (CoModes) is available on Rforge.

7.12. Mixture model for mixed kind of data

Participants: Christophe Biernacki, Matthieu Marbac Lourdelle, Vincent Vandewalle.

A mixture model of Gaussian copula allows to cluster mixed kind of data. Each component is composed by classical margins while the conditional dependencies between the variables is modeled by a Gaussian copula. The parameter estimation is performed by a Gibbs sampler. This work has been now accepted to an international journal [21]. Furthermore, an R package (MixCluster) is available on Rforge.

7.13. Degeneracy in multivariate Gaussian mixtures (complete data case)

Participant: Christophe Biernacki.

In the case of Gaussian mixtures, unbounded likelihood is an important theoretical and practical problem. Using the weak information that the latent sample size of each component has to be greater than the space dimension, a simple non-asymptotic stochastic lower bound on variances is derived. It is proved also that maximizing the likelihood under this data-driven constraint leads to consistent estimates. This work has been presented as an invited talk to the international workshop [28] and a paper for an international journal is been prepared.

This is a joined work with Gwënaelle Castellan of University of Lille.

7.14. Degeneracy in multivariate Gaussian mixtures (missing data case)

Participants: Christophe Biernacki, Vincent Vandewalle.

In the case of multivariate Gaussian mixtures, unbounded likelihood is an important theoretical and practical problem. However, in the case of missing data situations, this drawback is exacerbated for too reasons. Firstly, degeneracy frequence increases with missing data occurrence. Secondly, the EM dynamic is hardly detected since it implies linear grows of the log-likelihood, contrary to exponential grows in the complete data case, leading to computation waste and also high risk of erroneous estimates. Using the weak information that the latent sample size of each component (restricted to complete data) has to be greater than the space dimension, it is derived a simple contraint EM algorithm variant allowing to solve simultaneously both problems. This work has been presented to the international workshop [28] and a paper for an international journal is been prepared.

7.15. Data units selection in statistics

Participant: Christophe Biernacki.

Usually, the data unit definition is fixed by the practitioner but it can happen that it hesitates between several data unit options. In this context, it is highlighted that it is possible to embed data unit selection into a classical model selection principle. The problem is introduced in a regression context before to focus on the model-based clustering and co-clustering context, for data of different kinds (continuous, categorical, counting, ...). It has led to an invitation to an international workshop [29] and a preprint is being to be prepared.

It is a joint work with Alexandre Lourme from University of Bordeaux.

7.16. Label switching in Bayesian mixture model estimation

Participants: Christophe Biernacki, Benjamin Guedj, Vincent Vandewalle.

In the case of mixtures of distributions, it is well-known that the Bayesian posterior distribution is invariant to label switching, it means invariant to any renumbering of components. Consequences are important, typically leading to unuseful estimates like the posterior mean. Many attempts exist to solve this problem but it is advocated in this work that such a quest should be unfruitful since it is a direct consequence of the label non-identifiability of mixtures themselves. The present work proposes an original way to manage the label switching problem based on the Gibbs algorithm dynamic. The basic idea is to control the label switching probability along Gibbs iterations, controlled by both the sample size and the component overlap. An early version of this work has been presented as an invited talk to the international workshop [28].

7.17. Trade-off computation time and accuracy

Participants: Christophe Biernacki, Maxime Brunin, Alain Celisse.

Most estimates practically arise from algorithmic processes aiming at optimizing some standard, but usually only asymptotically relevant, criteria. Thus, the quality of the resulting estimate is a function of both the iteration number and also the involved sample size. An important question is to design accurate estimates while saving computation time, and we address it in the simplified context of linear regression here. Fixing the sample size, we focus on estimating an early stopping time of a gradient descent estimation process aiming at maximizing the likelihood. It appears that the accuracy gain of such a stopping time increases with the number of covariates, indicating potential interest of the method in real situations involving many covariates. A first version of this work has been presented to an international conference [27], and a preprint is being in progress.

7.18. Projection under pairwise control

Participant: Christophe Biernacki.

Visualization of high-dimensional and possibly complex (non continuous for instance) data onto a low-dimensional space may be difficult. Several projection methods have been already proposed for displaying such high-dimensional structures on a lower-dimensional space, but the information lost is not always easy to use. Here, a new projection paradigm is presented to describe a non-linear projection method that takes into account the projection quality of each projected point in the reduced space, this quality being directly available in the same scale as this reduced space. More specifically, this novel method allows a straightforward visualization data in R^2 with a simple reading of the approximation quality, and provides then a novel variant of dimensionality reduction.

This work is under revision in an international journal [37] and it has also been presented to an international conference [25].

It is a joint work with Hiba Alawieh and Nicolas Wicker, both from University of Lille.

7.19. Matching of descriptors evolving over time

Participants: Christophe Biernacki, Anne-Lise Bedenel.

In the web domain, and in particular for insurance comparison, data constantly evolve, implying that it is difficult to directly exploit them. For example, to do a classification, performing standard learning processes require data descriptor equal for both learning and test samples. Indeed, for answering to web surfer expectation, online forms whence data come from are regularly modified. So, features and data descriptors are also regularly modified. In this work, it is introduced a process to estimate and understand connections between transformed data descriptors. This estimated matching between descriptors will be a preliminary step before applying later classical learning methods. This work has been presented to a national conference [33], with international audience.

It is a joint work with Laetitia Jourdan, from University of Lille and Inria.

7.20. Real-time audio sources classification

Participants: Christophe Biernacki, Maxime Baelde.

Recent research on machine learning focuses on audio source identification in complex environments. They rely on extracting features from audio signals and use machine learning techniques to model the sound classes. However, such techniques are often not optimized for a real-time implementation and in multi-source conditions. It is proposed here a new real-time audio single-source classification method based on a dictionary of sound models (that can be extended to a multi-source setting). The sound spectrums are modeled with mixture models and form a dictionary. The classification is based on a comparison with all the elements of the dictionary by computing likelihoods and the best match is used as a result. It is found that this technique outperforms classic methods within a temporal horizon of 0.5s per decision (achieved 6% of errors on a database composed of 50 classes). Future works will focus on the multi-sources classification and reduce the computational load. This work has been accepted in 2016 to be presented in 2017 to an international conference in Signal Processing [32].

It is a joint work with Raphaël Greff, from the A-Volute company.

7.21. Model-Based Co-clustering for Ordinal Data

Participants: Christophe Biernacki, Julien Jacques.

A model-based coclustering algorithm for ordinal data is presented. This algorithm relies on the latent block model using the BOS model (Biernacki and Jacques, 2015, Stat. Comput.) for ordinal data and a SEM-Gibbs algorithm for inference. Numerical experiments on simulated data illustrate the efficiency of the inference strategy. This work has been presented to an international workshop [30] and also to a national conference with an international audience [35].

7.22. Computational and statistical trade-offs in change-point detection

Participants: Christophe Biernacki, Maxime Brunin, Alain Celisse.

The change-point detection problem aims to detect changes in the distribution of observations collected over the time between the instants 1,...,T in the offline context. These changes occur at some instants called change-points. Our method provides consistent estimates of the change-points obtained by the Kernel Binary Segmentation algorithm with stopping rule (KBS). Moreover, the proposed method has a lower complexity in time and in space than the Kernel Dynamic Programming (KDP). This work has been presented to a national conference with an international audience [34].

7.23. MixtComp software for full mixed data

Participants: Christophe Biernacki, Vincent Kubicki.

MixtComp (Mixture Computation) is an integration software from the MODAL team for model-based clustering of mixed data. Its computing core is written in C++ and is accessed through an R interface. Its architecture allows to easily and quickly integrate new univariate models (under the conditional independence assumption) as they are published. The first phase of development was the implementation of three basic models (Gaussian, Multinomial, Poisson) with the native management of partially observed data (including intervals). It now implements models related to ordinal data (2015), rank data (2015) and functional data (2016), still with missing or partially missing data. The code is developed internally, and has been field-tested through several contracted partnerships (see the section about contracts). It is now referenced in the BIL database and the APP. It is available through a new web interface, called MASSICCC at https://massiccc.lille.inria.fr/#/ (see also the dedicated section). MixtComp has been presented to an invited talk in October 2016 at the Academy of Sciences in Tunisia [26].

7.24. MASSICCC platform for SaaS software availability

Participants: Christophe Biernacki, Vincent Kubicki, Matthieu Marbac Lourdelle.

MASSICCC is a demonstration platform giving access through a SaaS (service as a software) concept to data analysis libraries developed at Inria. It allows to obtain results either directly through a website specific display (specific and interactive visual outputs) or through an R data object download. It started in October 2015 for two years and is common to the Modal team (Inria Lille) and the Select team (Inria Saclay). In 2016, two packages have been integrated: Mixmod and MixtComp (see the specific section about MixtComp). In 2017, it is planned to integrate the BlockCluster package. The MASSICCC platform gardually replaces the former BigStat platform available here: https://modal-research.lille.inria.fr/BigStat/. BigStat and MASSICCC have been both presented to an invited talk in October 2016 at the Academy of Sciences in Tunisia [26].

MASSICCC has led to a first short meeting in April 2016 in Lille for obtaining a feedback from company and academic users. Here is the link towards this event: Link. A second similar event is planned in February 2017 in Paris. Joint work with Jonas Renault and Josselin Demont (both at InriaTech).

The MASSICCC platform is available on https://massiccc.lille.inria.fr

7.25. CoModes package for correlated categorical variables

Participants: Christophe Biernacki, Matthieu Marbac Lourdelle, Vincent Vandewalle.

CoModes is an R package for model-based clustering of categorical data. In this package, the Conditional Modes Model (CMM), published in 2016 (Marbac et al, 2016), takes into account the main conditional dependencies between variables through particular modality crossings (so-called modes). CoModes performs the model selection and provides the best model according to the exact integrated likelihood criterion and the maximum likelihood estimates. It is available online on Rforge (https://r-forge.r-project.org/R/?group_id=1809).

7.26. MixCluster package for correlated mixed variables

Participants: Christophe Biernacki, Matthieu Marbac Lourdelle, Vincent Vandewalle.

MixCluster is an R package for model-based clustering of mixed data (continuous, binary, integer). In this package, the model, accepted for publication in 2016 [21], takes into account the main conditional dependencies between variables through Gaussian copula. Mixcluster performs the model selection and provides the best model according to Bayesian approaches. It is available online on Rforge (https://r-forge.r-project.org/R/?group_id=1939).

REALOPT Project-Team

7. New Results

7.1. Improving Branch-and-Price Methods

We have made progress on stabilization techniques and math-heuristics that are essential components for generic Branch-and-Price methods.

The convergence of a column generation algorithm can be improved in practice by using stabilization techniques. Smoothing and proximal methods based on penalizing the deviation from the incumbent dual solution have become standards of the domain. Interpreting column generation as cutting plane strategies in the dual problem, we have analyzed [29] the mechanisms on which stabilization relies. In particular, the link is established between smoothing and in-out separation strategies to derive generic convergence properties. For penalty function methods as well as for smoothing, we describe proposals for parameter self-adjusting schemes. Such schemes make initial parameter tuning less of an issue as corrections are made dynamically. Such adjustments also allow to adapt the parameters to the phase of the algorithm. Extensive test reports validate our self-adjusting parameter scheme and highlight their performances. Our results also show that using smoothing in combination with penalty function yields a cumulative effect on convergence speed-ups.

Math heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending MIP based heuristics, we have studied [18], [30] generic procedures to build primal solutions in the context of a branch-and-price approach. As the Dantzig-Wolfe reformulation of a problem is typically tighter than that of the original compact formulation, heuristics based on rounding its linear programing (LP) solution can be more competitive. We focus on the so-called diving methods that used re-optimization after each LP rounding. We explore combination with diversification- intensification paradigms such as Limited Discrepancy Search, sub-MIPing, relaxation induced neighborhood search, local branching, and strong branching. The dynamic generation of variables inherent to a column generation approach requires specific adaptation of heuristic paradigms. We manage to use simple strategies to get around these technical issues. Our numerical results on generalized assignment, cutting stock, and vertex coloring problems sets new benchmarks, highlighting the performance of diving heuristics as generic procedures in a column generation context and producing better solutions than state-of-the-art specialized heuristics in some cases.

7.2. Aggregation Techniques

We have developed [6] a general solution framework based on aggregation techniques to solve NP-Hard problems that can be formulated as a circulation model with specific side constraints. The size of the extended Mixed Integer Linear Programming formulation is generally pseudo-polynomial. To efficiently solve exactly these large scale models, we propose a new iterative aggregation and disaggregation algorithm. At each iteration, it projects the original model onto an aggregated one, producing an approximate model. The process iterates to refine the current aggregated model until the optimality is proved.

The computational experiments on two hard optimization problems (a variant of the vehicle routing problem and the cutting-stock problem) show that a generic implementation of the proposed framework allows us to outperform previous known methods.

We have applied this aggregation method to reduce the size of column generation (CG) models for covering problems in which the feasible subsets depend on a resource constraint [10]. The aggregation relies on a correlation between the resource consumption of the elements and the corresponding optimal dual values. The resulting aggregated dual model is a restriction of the original one, and it can be rapidly optimized to obtain a feasible dual solution. A primal bound can also be obtained by restricting the set of columns to those saturated by the dual feasible solution obtained by aggregation. The convergence is realized by iterative disaggregation until the gap is closed by the bounds. Computational results show the usefulness of our method for different cutting-stock problems. An important advantage is the fact that it can produce high-quality dual bounds much faster than the traditional lagrangian bound used in stabilized column generation.

7.3. Review of Algorithmic Enhancements for Benders Decomposition

In Benders decomposition approach to mixed integer programs, the optimization is carried in two stages: key first-stage decision variables are optimized using a polyhedral approximation of the full-blown problem projection, then a separation problem expressed in the second-stage variables is solved to check if the current first-stage solution is truly feasible, and otherwise, it produces a violated inequality. Such cutting-plane algorithms suffer from several drawbacks and may have very bad convergence rates. We have reviewed [23] the battery of approaches that have been proposed in the literature to address these drawbacks and to speed-up the algorithm. Our contribution consists in explaining these techniques in simple terms and unified notations, showing that in several cases, different proposals of the literature boil down to the same key ideas. We classify methods into specific initialization mode, stabilization techniques, strategies to select the separation point, and cut generation strategies. Where available, we highlight numerical benchmarks that have resulted from such enhancements.

7.4. Vehicle Routing Problems

Given a directed graph $G = (V, A)$, a cost function c associated with the arcs of A, and a set of precedence constraints $B \subset V \times V$, the Precedence Constrained Asymmetric Traveling Salesman Problem (PCATSP) seeks for a minimum cost Hamiltonian circuit, starting at node 1, and such that for each $(i, j) \in B$, the node i is visited before node j. There are many ways of modelling the ATSP and several for the PCATSP. In [20] we present new formulations for the two problems that can be viewed as resulting from combining precedence variable based formulations with network flow based formulations. Indeed, the former class of formulations permits to integrate linear ordering constraints. The motivating formulation for this work is a complicated and "ugly" formulation that results from the separation of generalized subtour elimination constraints presented. This so called "ugly" formulation exhibits, however, one interesting feature, namely the "disjoint subpaths" property that is further explored to create more complicated formulations that combine two (or three) "disjoint path" network flow based formulations and have a stronger linear programming bound. Some of these stronger formulations are related to the ones presented for the PCATSP and can be viewed as generalizations in the space of the precedence based variables. Several sets of projected inequalities in the space of the arc and precedence variables are obtained by projection from these network flow based formulations. Computational results for the ATSP and PCATSP evaluate the quality of the new models and inequalities.

The Dial-a-Ride Problem is a variant of the pickup and delivery problem with time windows, where the user inconvenience must be taken into account. In [17], ride time and customer waiting time are modeled through both constraints and an associated penalty in the objective function. We develop a column generation approach, dynamically generating feasible vehicle routes. Handling ride time constraints explicitly in the pricing problem solver requires specific developments. Our dynamic programming approach for pricing problem makes use of a heuristic dominance rule and a heuristic enumeration procedure, which in turns implies that our overall branch-and-price procedure is a heuristic. However, in practice our heuristic solutions are experimentally very close to exact solutions and our approach is numerically competitive in terms of computation times.

In [22], [21], we consider the problem of covering an urban area with sectors under additional constraints. We adapt the aggregation method to our column generation algorithm and focus on the problem of disaggregating the dual solution returned by the aggregated master problem.

7.5. Production Scheduling Problems

We have considered [7] the flowshop problem on two machines with sequence-independent setup times to minimize total completion time. Large scale network flow formulations of the problem are suggested together with strong Lagrangian bounds based on these formulations. To cope with their size, filtering procedures are developed. To solve the problem to optimality, we embed the Lagrangian bounds into two branch-and-bound algorithms. The best algorithm is able to solve all 100-job instances of our testbed with setup times and all 140-job instances without setup times, thus significantly outperforming the best algorithms in the literature.

In [9], we address a multi-activity tour scheduling problem with time varying demand. The objective is to compute a team schedule for a fixed roster of employees in order to minimize the over-coverage and the under-coverage of different parallel activity demands along a planning horizon of one week. Numerous complicating constraints are present in our problem: all employees are different and can perform several different activities during the same day-shift, lunch breaks and pauses are flexible, demand is given for 15 minutes periods. Employees have feasibility and legality rules to be satisfied, but the objective function does not account for any quality measure associated with each individual's schedule. More precisely, the problem mixes simultaneously days-off scheduling, shift scheduling, shift assignment, activity assignment, pause and lunch break assignment.

To solve this problem, we developed four methods: a compact Mixed Integer Linear Programming model, a branch-and-price like approach with a nested dynamic program to solve heuristically the subproblems, a diving heuristic and a greedy heuristic based on our subproblem solver. The computational results, based on both real cases and instances derived from real cases, demonstrate that our methods are able to provide good quality solutions in a short computing time. Our algorithms are now embedded in a commercial software, which is already in use in a mini-mart company.

7.6. Scheduling and Placement for HPC

With the complexification of the architecture of HPC nodes (multicores, non uniform memory access, GPU and accelerators), a recent trend in application development is to explicitely express the computations as a task graph, and rely on a specialized middleware stack to make scheduling decisions and implement them. Traditional algorithms used in this community are dynamic heuristics, to cope with the unpredictability of execution times. In [12], we analyze the performance of static and hybrid strategies, obtained by adding more static (resp. dynamic) features into dynamic (resp. static) strategies. Our conclusions are somehow unexpected in the sense that we prove that static-based strategies are very efficient, even in a context where performance estimations are not very good. We also present and generalize HeteroPrio, a semi-static resource-centric strategy based on the acceleration factors of tasks. In [19], we generalize this strategy to platforms with more than two types of resources. This allows to use intra-task parallelism by grouping several CPU cores together. In [27], we prove tight approximation ratios for HeteroPrio in the context of independent tasks, providing a theoretical insight to its good practical performance.

Another study [26] focuses on the memory-constrained case, where tasks may produce large data. A task can only be executed if all input and output data fit into memory, and a data can only be removed from memory after the completion of the task that uses it as an input data. There is a known, polynomial time algorithm [55] to minimize the peak memory used on one machine for the cases where the input graph is a rooted tree. We generalize in [26] to the variant where the input graph is a directed series-parallel graph, and propose a polynomial time algorithm. This allows to solve this practical problem in two important classes of applications.

In [13], we consider the static problem of data placement for matrix multiplication in heterogeneous machines, so as to optimize both load balancing and communication volume. This is modeled as a partitioning of a square into a set of zones of prescribed areas, while minimizing the overall size of their projections onto horizontal and vertical axes. We combine two ideas from the literature (recursive partitioning, and optimal solution structure for low number of processors) to obtain a non-rectangular recursive partitioning (NRRP), whose approximation ratio is $\frac{2}{\sqrt{3}} \simeq 1.15$, improving over the previous 1.25 ratio. Moreover, we observe on a large set of realistic platforms built from CPUs and GPUs that this proposed NRRP algorithm allows to achieve very efficient partitionings on all considered cases. In [14], we consider the generalization of this problem to the three dimensional case. We prove the NP-completeness of the problem, and propose a generalisation of NRRP with a $\left(\frac{5}{6}\right)^{\frac{2}{3}}$ approximation ratio.

7.7. Network Design Problems

The delivery of freight from manufacturing platforms to demand zones is often managed through one or more intermediate locations where storing, merging, transshipment and consolidation activities are performed. In [15], we design a Two-Echelon Distribution Network that helps synchronize different flows of product.

Under demand uncertainty, our model integrates decisions on the locations and the size of second echelon facilities an decisions on the flows assignment between the echelons, and on delivery routes to serve the demand zones.

In [8], we study the k-edge-connected L-hop-constrained network design problem. Given a weighted graph $G = (V, E)$, a set D of pairs of nodes, two integers $L \geq 2$ and $k \geq 2$, the problem consists in finding a minimum weight subgraph of G containing at least k edge-disjoint paths of length at most L between every pair $\{s, t\} \in D$. We consider the problem in the case where $L = 2$, 3 and $|D| \geq 2$. We first discuss integer programming formulations introduced in the literature. Then, we introduce new integer programming formulations for the problem that are based on the transformation of the initial undirected graph into directed layered graphs. We present a theoretical comparison of these formulations in terms of LP-bound. Finally, these formulations are tested using CPLEX and compared in a computational study for $k = 3, 4, 5$.

7.8. Strategic Planning of Phytosanitary treatments in Wineries

In [16], we consider planning phytosanitary treatments in a vineyard. We are given a set of diseases (or requests) that must be treated for each site. Product mixtures are defined by their composition of active components, and their duration of protective power for each request. Machines are available to spread the mixtures on the sites. The time horizon is divided in time periods. Sites are partitioned in sectors. The objective of the problem is to minimize the machine leasing costs, their travel cost to sectors and the costs related to the product use. To solve this problem, we use a column generation approach where the machine policy and the product order policy are pure master decisions, while treatment planning decisions are made in individual pricing subproblems associated with each site. We developed a dedicated dynamic program to solve the pricing subproblems.

7.9. Two-dimensional Guillotine-cut Bounded Knapsack Problem

The two-dimensional knapsack problem consists in packing a set of small rectangular items into a given large rectangle while maximizing the total reward associated with selected items. In [28], we restrict our attention to packings that emanate from a k-stage guillotine-cut process. We introduce a generic model where a knapsack solution is represented by a flow in a directed acyclic hypergraph. This hypergraph model derives from a forward labeling dynamic programming recursion that enumerates all non-dominated feasible cutting patterns. To reduce the hypergraph size, we make use of further dominance rules and a filtering procedure based on Lagrangian reduced costs fixing of hyperarcs. Our hypergraph model is (incrementally) extended to account for explicit bounds on the number of copies of each item. Our exact forward labeling algorithm is numerically compared to solving the max-cost flow model in the base hyper-graph with side constraints to model production bounds. Benchmarks are reported on instances from the literature and on datasets derived from a real-world application.

7.10. Matching-Based Allocation Strategies in Cloud Platforms

MapReduce is a well-know framework for distributing data-processing computations on parallel clusters. In MapReduce, a large computation is broken into small tasks that run in parallel on multiple machines, and scales easily to very large clusters of inexpensive commodity computers. Before the Map phase, the original dataset is first split into chunks, that are replicated (a constant number of times, usually 3) and distributed onto the computing nodes. During the Map phase, nodes request tasks and are allocated first tasks associated to local chunks (if any). Communications take place when requesting nodes do not hold any local chunk anymore. In [25], we provide the first complete theoretical data locality analysis of the Map phase of MapReduce, and more generally, for bag-of-tasks applications that behaves like MapReduce. We show that if tasks are homogeneous (in term of processing time), once the chunks have been replicated randomly on resources with a replication factor larger than 2, it is possible to find a priority mechanism for tasks that achieves a quasi-perfect number of communications using a sophisticated matching algorithm. In the more realistic case of heterogeneous processing times, we prove using an actual trace of a MapReduce server that this priority mechanism enables to complete the Map phase with significantly fewer communications, even on realistic distributions of task durations.

7.11. On Sets Avoiding Distance 1

In a joint work with C. Bachoc, T. Bellitto and P. Moustrou [11], we consider the maximum density of sets avoiding distance 1 in $\mathbb{R}^n$. Let $||.||$ be a norm of R^n and $G_{||.||}$ be the so-called unit distance graph with the points of R^n as vertex set and for edge set, the set of pairs $\{x, y\}$ such that $||x - y|| = 1$. An independent set of $G_{||.||}$ is said to avoid distance 1.

Let $||.||_E$ denote the Euclidean norm. For $n = 2$, the chromatic number of $G_{||.||_E}$ is still wide open: it is only known that $4 \leq \chi \left(G_{||.||_E}\right) \leq 7$ (Nelson, Isbell 1950). The *measurable* chromatic number χ_m of the graph $G_{||.||}$ is the minimal number of *measurable* stable sets of $G_{||.||}$ needed to cover all its vertices. Obviously, we have $\chi \left(G_{||.||_E}\right) \leq \chi_m \left(G_{||.||_E}\right)$. For $n = 2$, $5 \leq \chi_m \left(G_{||.||_E}\right)$ (Falconer 1981).

Let $m_1 \left(G_{||.||}\right)$ denote the maximum density of a measurable set avoiding distance 1. We have $\frac{1}{m_1\left(G_{||.||}\right)} \leq \chi_m \left(G_{||.||}\right)$. We study the maximum density m_1 for norms defined by polytopes: if P is a centrally symmetric polytope and x is a point of R^n, $||x||_P$ is the smallest positive real t such that $x \in tP$. Polytope norms include some usual norms such as the L^1 and L^∞ norms.

If P tiles the space by translation, then it is easy to see that $m_1 \left(G_{||.||_P}\right) \geq \frac{1}{2^n}$. C. Bachoc and S. Robins conjectured that equality always holds. We show that this conjecture is true for $n = 2$ and for some polytopes in higher dimensions.

SELECT Project-Team

6. New Results

6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, Serge Cohen, Pascal Massart, Sylvain Arlot, Jean-Michel Poggi, Kevin Bleakley.

The well-documented and consistent variable selection procedure in model-based cluster analysis and classification that Cathy Maugis (INSA Toulouse) designed during her PhD thesis in SELECT, makes use of stepwise algorithms which are painfully slow in high dimensions. In order to circumvent this drawback, Gilles Celeux, in collaboration with Mohammed Sedki (Université Paris XI) and Cathy Maugis), have proposed to sort variables using a lasso-like penalization adapted to the Gaussian mixture model context. Using this ranking to select variables, they avoid the combinatory problem of stepwise procedures. The performances on challenging simulated and real data sets are similar to the standard procedure, with a CPU time divided by a factor of more than a hundred.

In collaboration with Jean-Michel Marin (Université de Montpellier) and Olivier Gascuel (LIRMM), Gilles Celeux has continued research aiming to select a short list of models rather a single model. This short list is declared to be compatible with the data using a p-value derived from the Kullback-Leibler distance between the model and the empirical distribution. Furthermore, the Kullback-Leibler distances at hand are estimated through nonparametric and parametric bootstrap procedures. Different strategies are compared through numerical experiments on simulated and real data sets. This year their method has been compared favorably to competing methods.

Sylvain Arlot, in collaboration with Damien Garreau (Inria Paris, Sierra team), studied the kernel change-point algorithm (KCP) proposed by Arlot, Celisse and Harchaoui, that aims at locating an unknown number of change-points in the distribution of a sequence of independent data taking values in an arbitrary set. The change-points are selected by model selection with a penalized kernel empirical criterion. They provide a non-asymptotic result showing that, with high probability, the KCP procedure retrieves the correct number of change-points, provided that the constant in the penalty is well-chosen; in addition, KCP estimates the change-points location at the minimax rate $\log(n)/n$. As a consequence, when using a characteristic kernel, KCP detects all kinds of change in the distribution (not only changes in the mean or the variance), and it is able to do so for complex structured data (not necessarily in $\mathbb{R}^d$). Most of the analysis is conducted assuming that the kernel is bounded; part of the results can be extended when we only assume a finite second-order moment.

Emilie Devijver, Yannig Goude and Jean-Michel Poggi have proposed a new methodology for customer segmentation, in the context of load profiles in energy consumption. The method is based on high-dimensional regression models which perform clustering and model selection at the same time. They have focused on uncovering classes corresponding to different regression models, and compute clustering and model identification in each cluster simultaneously. They have shown the feasibility of the approach on a real data set of Irish customers. Benjamin Goehry is completing a thesis co-supervised by P. Massart and J-M. Poggi, aiming at extending this scheme by introducing the use of time series forecasting models adapted to each cluster.

J-M. Poggi, with J. Cugliari, Y. Goude, have proposed building clustering tools useful for forecasting load consumption. The idea is to disaggregate the global signal in such a way that the sum of disaggregated forecasts significantly improves the prediction of the whole global signal. The strategy has three steps: first they cluster curves defining super-consumers, then they build a hierarchy of partitions from which the best one is selected with respect to a disaggregated forecast criterion. The proposed strategy is applied to a dataset of individual consumers from the French electricity provider EDF.

V. Thouvenot and J-M. Poggi, with A. Pichavant, A. Antoniadis, Y. Goude, consider electricity forecasting using multi-stage estimators of nonlinear additive models. An automatic procedure for variable selection is used to correct middle term forecasting errors for short term forecasting. An application to the EDF customer load demand at an aggregate level is considered as well as an application on load demand from the GEFCom 2012 competition; this is a local application.

6.2. Estimator selection

Participants: Claire Lacour, Pascal Massart.

Estimator selection has become a crucial issue in nonparametric estimation. Two widely used methods are penalized empirical risk minimization (such as penalized log-likelihood estimation) and pairwise comparison (such as Lepski's method). C. Lacour, P. Massart and V. Rivoirard have developed a new method for bandwidth selection which is in some sense intermediate between these two main methods mentioned above, and is called "Penalized Comparison to Overfitting". They have first provided some theoretical results (oracle bounds, minimal penalty) within the framework of kernel density estimation, which leads to some fully data-driven selection strategies. Currently, S. Varet is implementing this method, making a thorough comparison with other selection methods, and tackling the multivariate case. Theoretical work is also in progress, in order to expand the method to other loss functions, such as the Hellinger loss.

6.3. Statistical learning methodology and theory

Participants: Gilles Celeux, Christine Keribin, Michel Prenat, Kaniav Kamary, Sylvain Arlot, Benjamin Auder, Jean-Michel Poggi, Neska El Haouij, Kevin Bleakley.

Gaussian graphical models are widely used to infer and visualize networks of dependencies between continuous variables. However, inferring the graph is difficult when the sample size is small compared to the number of variables. To reduce the number of parameters to estimate in the model, the past PhD. students Emilie Devijver (supervisors: Pascal Massart and Jean-Michel Poggi) and Mélina Gallopin (supervisor: Gilles Celeux) proposed a non-asymptotic model selection procedure supported by strong theoretical guarantees based on an oracle inequality and a minimax lower bound. The covariance matrix of the model is approximated by a block-diagonal matrix. The structure of this matrix is detected by thresholding the sample covariance matrix, where the threshold is selected using the slope heuristic. Based on the block-diagonal structure of the covariance matrix, the estimation problem is divided into several independent problems: subsequently, the network of dependencies between variables is inferred using the graphical lasso algorithm in each block. The performance of the procedure has been illustrated on simulated data. An application to a real gene expression dataset with a limited sample size has been achieved: the dimension reduction allows attention to be objectively focused on interactions among smaller subsets of genes, leading to a more parsimonious and interpretable modular network. This work has been accepted for publication in the *Journal of the American Statistical Association*.

J-M. Poggi, with A. Bar-Hen, have focused on individual observation diagnosis issues for graphical models. The use of an influence measure is a classical diagnostic method to measure the perturbation induced by single elements. The stability issue is here considered using jackknife. For a given graphical model, tools to perform diagnosis on observations are provided. In the second step, a filtering of the dataset to obtain a stable network is proposed.

Latent Block Models (LBM) are a model-based method to cluster simultaneously the d columns and n rows of a data matrix. The Blockcluster package estimates such LBMs. Parameter estimation in LBM is a difficult and multifaceted problem. Although various estimation strategies have been proposed and are now well-understood empirically, theoretical guarantees about their asymptotic behavior is rather rare. Christine Keribin, in collaboration with Mahendra Mariadassou (INRA) and Vincent Brault (Université de Grenoble) have shown that under some mild conditions on the parameter space, and in an asymptotic regime where $\log(d)/n$ and $\log(n)/d$ go to 0 when n and d go to $+\infty$, (1) the maximum likelihood estimate of the complete model (with known labels) is consistent and (2) the log-likelihood ratios are equivalent under the complete and observed (with unknown labels) models. This equivalence allows us to transfer the asymptotic consistency to the maximum likelihood estimate under the observed model. Moreover, the variational estimator is also consistent. These results extends the results of Bickel et al. (2013) on stochastic block models, and detail the case where the parameter exhibits symmetry.

For the same LBM, Valérie Robert and Yann Vasseur have extended the popular Adjusted Rand Index (ARI) to the task of simultaneous clustering of the rows and columns of a given matrix. This new index, called the Coclustering Adjusted Rand Index (CARI), overcomes the label switching phenomenon while remaining useful and competitive with respect to other indices. Indeed, partitions with high numbers of clusters can be considered, and no convention is required when the numbers of clusters in partitions are different. They are now exploring links with other indices.

Gilles Celeux continued his collaboration with Jean-Patrick Baudry on model-based clustering. This year, they proposed to consider the model selection criterion ICL as a validity index. They show how it can be coupled with a null model of homogeneity focusing on clustering. This null model, which includes the Gaussian distributions, can be difficult to analyze. They find an explicit representation for simple models and show how the parametric bootstrap test can be applied in such situations. In more general situations, they propose a solution for applying this approach involving an "acceptance-rejection" procedure which explores the parameter space to approximate the maximum likelihood estimator inside the null model of homogeneity. The uncovering of this null model highlights the notion of class underlying ICL, and confirms the results of earlier results which show that ICL is consistent for a loss function taking clustering into account.

In collaboration with Arthur White and Jason Wyse (Trinity College, Dublin) Gilles Celeux has evaluated for multivariate Poisson mixture models the performance of a greedy search method compared to the expectation maximization (EM) algorithm, to optimize the ICL model selection criterion, which can be computed exactly for such models. It appears that EM gives often slightly better results, but the greedy search is computationally is more efficient.

The Dutch and French schools of data analysis differ in their approaches to the question: How does one understand and summarize the information contained in a data set? Julie Josse, in collaboration with François Husson (Agro Rennes) and Gibert Saporta (CNAM, Paris), explored the shared factors and differences between the schools, with a focus on methods dedicated to the analysis of categorical data, which are known either as homogeneity analysis (HOMALS) or multiple correspondence analysis (MCA). MCA is a dimension-reduction method which plays a large role in the analysis of tables with categorical nominal variables such as survey data. Though it is usually motivated and derived using geometric considerations, they proved that it amounts to a single proximal Newton step of a natural bilinear exponential family model for categorical data: the multinomial logit bilinear model. They compared and contrasted the behavior of MCA with that of the model on simulations, and discussed new insights into the properties of both exploratory multivariate methods and their cognate models. The main conclusion is to recommend approximating the multilogit model parameters using MCA. Indeed, estimating the parameters of the model is not a trivial task, whereas MCA has the great advantage of being easily solved by a singular value decomposition, as well as being scalable to large datasets.

Julie Josse, with Sobczyk and Bogdan, have discussed the problem of estimating the number of principal components in Principal Components Analysis (PCA). They address this issue by presenting an approximate Bayesian approach based on Laplace approximation, and introduce a general method for building the model selection criteria, called PEnalized SEmi-integrated Likelihood (PESEL). This general framework encompasses a variety of existing approaches based on probabilistic models, like e.g., Bayesian Information Criterion for the Probabilistic PCA (PPCA), and allows for construction of new criteria, depending on the size of the data set at hand. Specifically, they define PESEL when the number of variables substantially exceeds the number of observations. Numerical simulations show that PESEL-based criteria can be quite robust against deviations from probabilistic model assumptions. Selected PESEL-based criteria for estimation of the number of principal components are implemented in the R package varclust, which is available on Github.

Gillies Celeux and Julie Josse have started research on missing data for model-based clustering in collaboration with Christophe Biernacki (Modal, Inria Lille). The aim of this research is to propose appropriate and efficient tools for the packages Mixmod and Mixtcomp.

In collaboration with Jean-Michel Marin (Université de Montpellier) and Christian Robert (Université Paris 9-Dauphine), Gilles Celeux and Kaniav Kamary investigated the ability of Bayesian inference to properly estimate the parameters of Gaussian mixtures in high dimensions. Their study shows how the choice of the prior distributions is important. In particular, independent prior distributions give much better performances. Moreover, when the dimension d becomes very large (say $d > 40$) Bayesian inference becomes questionable. The results of this study will be gathered in a chapter of a book on mixture models that Gilles Celeux is preparing with Christian Robert and Sylvia Fruhwirth Schnatter.

Sylvain Arlot, in collaboration with Robin Genuer (ISPED), studied the reasons why random forests work so well in practice. Focusing on the problem of quantifying the impact of each ingredient of random forests on their performance, they showed that such a quantification is possible for a simple pure forest, leading to conclusions that could apply more generally. Then, they considered "hold-out" random forests, which are a good midpoint between "toy" pure forests and Breiman's original random forests.

J.-M. Poggi and N. El Haouij (with R. Ghozi, S. Sevestre Ghalila and M. Jaïdane) provide a random forest-based method for the selection of physiological functional variables in order to classify stress levels during a real-world driving experience. The contribution of this study is twofold: on the methodological side, it considers physiological signals as functional variables and offers a procedure for data processing and variable selection. On the applied side, the proposed method provides a "blind" procedure of driver's stress level classification that does not depend on expert-based studies of physiological signals.

J-M. Poggi (with R. Genuer, C. Tuleau-Malot, N. Villa-Vialaneix), have focused on random forests in Big Data classification problems, and have performed a review of available proposals about random forests in parallel environments as well as on online random forests. Three variants involving subsampling, Big Data-bootstrap and MapReduce respectively are tested on two massive datasets, one simulated one, and the other, real-world data.

B. Auder and J-M. Poggi (with M. Bobbia, B. Portier) have tested some methods for sequential aggregation for forecasting PM10 concentrations for the next day, in the context of air quality monitoring in Normandy (France). The main originality is that the set of experts contains at the same time statistical models built by means of various methods and groups of predictors, as well as experts coming from deterministic chemical models of prediction. The obtained results show that such a strategy clearly improves the performances of the best expert both in terms of prediction errors and in terms of alerts. What is more, it obtains, for the non-convex weighting strategy, the "unbiasedness" of observed-forecasted scatterplots, which is extremely difficult to obtain.

J-M. Poggi (with A. Antoniadis, I. Gijbels, S. Lambert-Lacroix) have considered the joint estimation and variable selection for mean and dispersion in proper dispersion models. They used recent results on Bregman divergence for establishing theoretical results for the proposed estimators in fairly general settings, and also studied variable selection when there is a large number of covariates, with this number possibly tending to infinity with the sample size. The proposed estimation and selection procedure is investigated via a simulation study, and illustrated via some real data applications.

6.4. Estimation for conditional densities in high dimension

Participants: Claire Lacour, Jeanne Nguyen.

Jeanne Nguyen is working on estimation for conditional densities in high dimension. Much more informative than the regression function, conditional densities are of high interest in recent methods, particularly in the Bayesian framework (studying the posterior distribution). Considering a specific family of kernel estimators, she is studying a greedy algorithm for selecting the bandwidth. Her method addresses several issues: avoiding the curse of high dimensionality under some suitably defined sparsity conditions, being computationally efficient using iterative procedures, and early variable selection, providing theoretical guarantees on the minimax risk.

6.5. Reliability

Participants: Gilles Celeux, Florence Ducros, Patrick Pamphile.

Since June 2015, in the framework of a CIFRE convention with Nexter, Florence Ducros has begun a thesis on the modeling of aging of vehicles, supervised by Gilles Celeux and Patrick Pamphile. This thesis should lead to designing an efficient maintenance strategy according to vehicle use profiles. It involves the estimation of mixtures and competing risk models in a highly-censored setting. Moreover, she can deduce from these models operational tools to estimate the number of spare parts to be stocked in a given period. These tools are defined to take vehicle use patterns into account.

6.6. Statistical analysis of genomic data

Participants: Gilles Celeux, Mélina Gallopin, Christine Keribin, Yann Vasseur, Kevin Bleakley.

The subject of Yann Vasseur's PhD Thesis, supervised by Gilles Celeux and Marie-Laure Martin-Magniette (INRA URGV), is the inference of a regulatory network for Transcriptions Factors (TFs), which are specific genes, of *Arabidopsis thaliana*. For this, a transcriptome dataset with a similar number of TFs and statistical units is available. The first aim consists of reducing the dimension of the network to avoid high-dimensional difficulties. Representing this network with a Gaussian graphical model, the following procedure has been defined:

1. *Selection step*: choose the set of TF regulators (supports) of each TF.
2. *Classification step*: deduce co-factor groups (TFs with similar expression levels) from these supports.

Thus, the reduced network would be built on the co-factor groups. Currently, several selection methods based on Gauss-LASSO and resampling procedures have been applied to the dataset. The study of stability and parameter calibration of these methods is in progress. The TFs are clustered with the Latent Block Model into a number of co-factor groups, selected with BIC or the exact ICL criterion. Since these models are built in an ad hoc way, Yann Vasseur has defined complex simulation tools to asses their performances in a proper way.

In a collaboration with Marie-Laure Martin-Magniette, Cathy Maugis and Andrea Rau, Gilles Celeux has studied gene expression obtained from high-throughput sequencing technology. The focus is on the question of clustering gene expression profiles as a means to discover groups of co-expressed genes. A Poisson mixture model is proposed, using a rigorous framework for parameter estimation, as well as for the choice of the appropriate number of clusters. They illustrate co-expression analyses using this approach on two real RNA-seq datasets. A set of simulation studies also compares the performance of the proposed model with that of several related approaches developed to cluster RNA-seq and serial analysis of gene expression data. The proposed method is implemented in the open-source R package `HTSCluster`, available on CRAN. It can now be compared with Gaussian mixtures obtained after relevant data transformations. Moreover, the performance of `HTSCluster` is compared with $k$means-like algorithms using the χ^2 distance.

In collaboration with Benno Schwikowski, Iryna Nikolayeva and A Anavaj Sakuntabhai (Pasteur Institute, Paris), Kevin Bleakley works on using 2-d isotonic regression to predict dengue fever severity at hospital arrival using high-dimensional microarray gene expression data. Important marker genes for dengue severity have been detected, some of which now have been validated in external lab trials.

6.7. Model based-clustering for pharmacovigilance data

Participants: Gilles Celeux, Christine Keribin, Valérie Robert.

In collaboration with Pascale Tubert-Bitter, Ismael Ahmed and Mohamed Sedki, Gilles Celeux and Christine Keribin have started research concerning the detection of associations between drugs and adverse events in the framework of the PhD of Valerie Robert. At first, this team developed model-based clustering inspired by latent block models, which consists of co-clustering rows and columns of two binary tables, imposing the same row ranking. This enables it to highlight subgroups of individuals sharing the same drug profile, and subgroups of adverse effects and drugs with strong interactions. Furthermore, some sufficient conditions are provided to obtain identifiability of the model, and some results are shown for simulated data. The exact ICL criterion has been extended to this double block latent model. Through computer experiments, Valérie Robert has demonstrated the interest of the proposed model, compared with standard contingency table analysis, to detect co-prescription and masking effects.

6.8. Statistical rating and ranking of scientific journals

Participants: Gilles Celeux, Julie Josse, Simon Grah.

In collaboration with Jean-Louis Foulley (université of Montpellier), Gilles Celeux and Julie Josse have started research on statistical rating and ranking of scientific journals. This research was the subject of the internship of Simon Grah (Université Paris-Sud). Simon Grah compared many models on a set of 47 statistical journals. His study showed that the Row-Column (RC) models appears to be the most relevant. In the future, Bayesian inference for different approaches, including PageRank, will be considered.

SEQUEL Project-Team

7. New Results

7.1. Decision-making Under Uncertainty

7.1.1. Reinforcement Learning

Analysis of Classification-based Policy Iteration Algorithms, [20]

We introduce a variant of the classification-based approach to policy iteration which uses a cost-sensitive loss function weighting each classification mistake by its actual regret, that is, the difference between the action-value of the greedy action and of the action chosen by the classifier. For this algorithm, we provide a full finite-sample analysis. Our results state a performance bound in terms of the number of policy improvement steps, the number of rollouts used in each iteration, the capacity of the considered policy space (classifier), and a capacity measure which indicates how well the policy space can approximate policies that are greedy with respect to any of its members. The analysis reveals a tradeoff between the estimation and approximation errors in this classification-based policy iteration setting. Furthermore it confirms the intuition that classification-based policy iteration algorithms could be favorably compared to value-based approaches when the policies can be approximated more easily than their corresponding value functions. We also study the consistency of the algorithm when there exists a sequence of policy spaces with increasing capacity.

Reinforcement Learning of POMDPs using Spectral Methods, [23]

We propose a new reinforcement learning algorithm for partially observable Markov decision processes (POMDP) based on spectral decomposition methods. While spectral methods have been previously employed for consistent learning of (passive) latent variable models such as hidden Markov models, POMDPs are more challenging since the learner interacts with the environment and possibly changes the future observations in the process. We devise a learning algorithm running through episodes, in each episode we employ spectral techniques to learn the POMDP parameters from a trajectory generated by a fixed policy. At the end of the episode, an optimization oracle returns the optimal memoryless planning policy which maximizes the expected reward based on the estimated POMDP model. We prove an order-optimal regret bound w.r.t. the optimal memoryless policy and efficient scaling with respect to the dimensionality of observation and action spaces.

Bayesian Policy Gradient and Actor-Critic Algorithms, [15]

Policy gradient methods are reinforcement learning algorithms that adapt a parameterized policy by following a performance gradient estimate. Many conventional policy gradient methods use Monte-Carlo techniques to estimate this gradient. The policy is improved by adjusting the parameters in the direction of the gradient estimate. Since Monte-Carlo methods tend to have high variance, a large number of samples is required to attain accurate estimates, resulting in slow convergence. In this paper, we first propose a Bayesian framework for policy gradient, based on modeling the policy gradient as a Gaussian process. This reduces the number of samples needed to obtain accurate gradient estimates. Moreover, estimates of the natural gradient as well as a measure of the uncertainty in the gradient estimates, namely, the gradient covariance, are provided at little extra cost. Since the proposed Bayesian framework considers system trajectories as its basic observable unit, it does not require the dynamics within trajectories to be of any particular form, and thus, can be easily extended to partially observable problems. On the downside, it cannot take advantage of the Markov property when the system is Markovian. To address this issue, we proceed to supplement our Bayesian policy gradient framework with a new actor-critic learning model in which a Bayesian class of non-parametric critics, based on Gaussian process temporal difference learning, is used. Such critics model the action-value function as a Gaussian process, allowing Bayes' rule to be used in computing the posterior distribution over action-value functions, conditioned on the observed data. Appropriate choices of the policy parameterization and of the prior covariance (kernel) between action-values allow us to obtain closed-form expressions for the posterior distribution of the gradient of the expected return with respect to the policy parameters. We perform detailed experimental comparisons of the proposed Bayesian policy gradient and actor-critic algorithms with classic Monte-Carlo based policy gradient methods, as well as with each other, on a number of reinforcement learning problems.

7.1.2. Multi-arm Bandit Theory

Improved Learning Complexity in Combinatorial Pure Exploration Bandits, [32]

We study the problem of combinatorial pure exploration in the stochastic multi-armed bandit problem. We first construct a new measure of complexity that provably characterizes the learning performance of the algorithms we propose for the fixed confidence and the fixed budget setting. We show that this complexity is never higher than the one in existing work and illustrate a number of configurations in which it can be significantly smaller. While in general this improvement comes at the cost of increased computational complexity, we provide a series of examples , including a planning problem, where this extra cost is not significant.

Online learning with noisy side observations, [43]

We propose a new partial-observability model for online learning problems where the learner, besides its own loss, also observes some noisy feedback about the other actions, depending on the underlying structure of the problem. We represent this structure by a weighted directed graph, where the edge weights are related to the quality of the feedback shared by the connected nodes. Our main contribution is an efficient algorithm that guarantees a regret of $O(\sqrt{\alpha * T})$ after T rounds, where α * is a novel graph property that we call the effective independence number. Our algorithm is completely parameter-free and does not require knowledge (or even estimation) of α *. For the special case of binary edge weights, our setting reduces to the partial-observability models of Mannor & Shamir (2011) and Alon et al. (2013) and our algorithm recovers the near-optimal regret bounds.

Online learning with Erdös-Rényi side-observation graphs, [42]

We consider adversarial multi-armed bandit problems where the learner is allowed to observe losses of a number of arms beside the arm that it actually chose. We study the case where all non-chosen arms reveal their loss with an unknown probability rt, independently of each other and the action of the learner. Moreover, we allow rt to change in every round t, which rules out the possibility of estimating rt by a well-concentrated sample average. We propose an algorithm which operates under the assumption that rt is large enough to warrant at least one side observation with high probability. We show that after T rounds in a bandit problem with N arms, the expected regret of our algorithm is of order O(sqrt(sum(t=1)T (1/rt) log N)), given that rt less than log T / (2N-2) for all t. All our bounds are within logarithmic factors of the best achievable performance of any algorithm that is even allowed to know exact values of rt.

Revealing graph bandits for maximizing local influence, [27]

We study a graph bandit setting where the objective of the learner is to detect the most influential node of a graph by requesting as little information from the graph as possible. One of the relevant applications for this setting is marketing in social networks, where the marketer aims at finding and taking advantage of the most influential customers. The existing approaches for bandit problems on graphs require either partial or complete knowledge of the graph. In this paper, we do not assume any knowledge of the graph, but we consider a setting where it can be gradually discovered in a sequential and active way. At each round, the learner chooses a node of the graph and the only information it receives is a stochastic set of the nodes that the chosen node is currently influencing. To address this setting, we propose BARE, a bandit strategy for which we prove a regret guarantee that scales with the detectable dimension, a problem dependent quantity that is often much smaller than the number of nodes.

Algorithms for Differentially Private Multi-Armed Bandits, [50]

We present differentially private algorithms for the stochastic Multi-Armed Bandit (MAB) problem. This is a problem for applications such as adaptive clinical trials, experiment design, and user-targeted advertising where private information is connected to individual rewards. Our major contribution is to show that there exist (ϵ, δ) differentially private variants of Upper Confidence Bound algorithms which have optimal regret, $O(\epsilon^{-1} + \log T)$. This is a significant improvement over previous results, which only achieve poly-log regret

$O(\epsilon^{-2} \log^2 T)$, because of our use of a novel interval-based mechanism. We also substantially improve the bounds of previous family of algorithms which use a continual release mechanism. Experiments clearly validate our theoretical bounds.

On the Complexity of Best Arm Identification in Multi-Armed Bandit Models, [17]

The stochastic multi-armed bandit model is a simple abstraction that has proven useful in many different contexts in statistics and machine learning. Whereas the achievable limit in terms of regret minimization is now well known, our aim is to contribute to a better understanding of the performance in terms of identifying the m best arms. We introduce generic notions of complexity for the two dominant frameworks considered in the literature: fixed-budget and fixed-confidence settings. In the fixed-confidence setting, we provide the first known distribution-dependent lower bound on the complexity that involves information-theoretic quantities and holds when m is larger than 1 under general assumptions. In the specific case of two armed-bandits, we derive refined lower bounds in both the fixed-confidence and fixed-budget settings, along with matching algorithms for Gaussian and Bernoulli bandit models. These results show in particular that the complexity of the fixed-budget setting may be smaller than the complexity of the fixed-confidence setting, contradicting the familiar behavior observed when testing fully specified alternatives. In addition, we also provide improved sequential stopping rules that have guaranteed error probabilities and shorter average running times. The proofs rely on two technical results that are of independent interest : a deviation lemma for self-normalized sums (Lemma 19) and a novel change of measure inequality for bandit models (Lemma 1).

Optimal Best Arm Identification with Fixed Confidence, [33]

We give a complete characterization of the complexity of best-arm identification in one-parameter bandit problems. We prove a new, tight lower bound on the sample complexity. We propose the 'Track-and-Stop' strategy, which we prove to be asymptotically optimal. It consists in a new sampling rule (which tracks the optimal proportions of arm draws highlighted by the lower bound) and in a stopping rule named after Chernoff, for which we give a new analysis.

On Explore-Then-Commit Strategies, [35]

We study the problem of minimising regret in two-armed bandit problems with Gaussian rewards. Our objective is to use this simple setting to illustrate that strategies based on an exploration phase (up to a stopping time) followed by exploitation are necessarily suboptimal. The results hold regardless of whether or not the difference in means between the two arms is known. Besides the main message, we also refine existing deviation inequalities, which allow us to design fully sequential strategies with finite-time regret guarantees that are (a) asymptotically optimal as the horizon grows and (b) order-optimal in the minimax sense. Furthermore we provide empirical evidence that the theory also holds in practice and discuss extensions to non-gaussian and multiple-armed case.

7.1.3. Recommendation systems

Scalable explore-exploit Collaborative Filtering, [39]

Recommender Systems (RS) aim at suggesting to users one or several items in which they might have interest. These systems have to update themselves as users provide new ratings, but also as new users/items enter the system. While this adaptation makes recommendation an intrinsically sequential task, most researches about RS based on Collaborative Filtering are omitting this fact, as well as the ensuing exploration/exploitation dilemma: should the system recommend items which bring more information about the users (explore), or should it try to get an immediate feedback as high as possible (exploit)? Recently, a few approaches were proposed to solve that dilemma, but they do not meet requirements to scale up to real life applications which is a crucial point as the number of items available on RS and the number of users in these systems explode. In this paper, we present an explore-exploit Collaborative Filtering RS which is both efficient and scales well. Extensive experiments on some of the largest available real-world datasets show that the proposed approach performs accurate personalized recommendations in less than a millisecond per recommendation, which makes it a good candidate for true applications.

Large-scale Bandit Recommender System, [38] The main target of Recommender Systems (RS) is to propose to users one or several items in which they might be interested. However, as users provide more feedback, the recommendation process has to take these new data into consideration. The necessity of this update phase makes recommendation an intrinsically sequential task. A few approaches were recently proposed to address this issue, but they do not meet the need to scale up to real life applications. In this paper , we present a Collaborative Filtering RS method based on Matrix Factorization and Multi-Armed Bandits. This approach aims at good recommendations with a narrow computation time. Several experiments on large datasets show that the proposed approach performs personalized recommendations in less than a millisecond per recommendation.

Sequential Collaborative Ranking Using (No-)Click Implicit Feedback, [40]

We study Recommender Systems in the context where they suggest a list of items to users. Several crucial issues are raised in such a setting: first, identify the relevant items to recommend; second, account for the feedback given by the user after he clicked and rated an item; third, since new feedback arrive into the system at any moment, incorporate such information to improve future recommendations. In this paper, we take these three aspects into consideration and present an approach handling click/no-click feedback information. Experiments on real-world datasets show that our approach outperforms state of the art algorithms.

Hybrid Recommender System based on Autoencoders, [49]

A standard model for Recommender Systems is the Matrix Completion setting: given partially known matrix of ratings given by users (rows) to items (columns), infer the unknown ratings. In the last decades, few attempts where done to handle that objective with Neural Networks, but recently an architecture based on Autoencoders proved to be a promising approach. In current paper, we enhanced that architecture (i) by using a loss function adapted to input data with missing values, and (ii) by incorporating side information. The experiments demonstrate that while side information only slightly improve the test error averaged on all users/items, it has more impact on cold users/items.

Compromis exploration-exploitation pour système de recommandation à grande échelle, [53]

Les systèmes de recommandation recommandent à des utilisateurs un ou des produits qui pourraient les intéresser. La recommandation se fonde sur les retours des utilisateurs par le passé, lors des précédentes recommandations. La recommandation est donc un problème séquentiel et le système de recommandation recommande (i) pour obtenir une bonne récompense, mais aussi (ii) pour mieux cerné l'utilisateur/les produits et ainsi obtenir de meilleures récompenses par la suite. Quelques approches récentes ciblent ce double objectif mais elles sont trop gourmandes en temps de calcul pour s'appliquer à certaines applications de la vie réelle. Dans cet article, nous présentons un système de recommandation fondé sur la factorisation de matrice et les bandits manchots. Plusieurs expériences sur de grandes base de données montrent que l'approche proposée fournit de bonnes recommendations en moins d'une milli-seconde par recommandation.

Filtrage Collaboratif Hybride avec des Auto-encodeurs, [54]

Le filtrage collaboratif (CF) exploite les retours des utilisateurs pour leur fournir des recommandations personnalisées. Lorsque ces algorithmes ont accès à des informations complémentaires, ils ont de meilleurs résultats et gèrent plus efficacement le démarrage à froid. Bien que les réseaux de neurones (NN) remportent de nombreux succès en traitement d'images, ils ont reçu beaucoup moins d'attention dans la communauté du CF. C'est d'autant plus surprenant que les NN apprennent comme les algorithme de CF une représentation latente des données. Dans cet article, nous introduisons une architecture de NN adaptée au CF (nommée CFN) qui prend en compte la parcimonie des données et les informations complémentaires. Nous montrons empiriquement sur les bases de données MovieLens et Douban que CFN bât l'état de l'art et profite des informations complémentaires. Nous fournissons une implémentation de l'algorithme sous forme d'un plugin pour Torch.

7.1.4. Nonparametric statistics of time series

Things Bayes can't do, [48]

The problem of forecasting conditional probabilities of the next event given the past is consideredin a general probabilistic setting. Given an arbitrary (large, uncountable) set C of predictors, we would like to construct a single predictor that performs asymptotically as well as the best predictor in C, on any data. Here we show that there are sets C for which such predictors exist, but none of them is a Bayesian predictor with a prior concentrated on C.In other words, there is a predictor with sublinear regret, but every Bayesian predictor must have a linear regret. This negative finding is in sharp contrast with previous resultsthat establish the opposite for the case when one of the predictors in C achieves asymptotically vanishing error.In such a case, if there is a predictor that achieves asymptotically vanishing error for any measure in C, then there is a Bayesian predictor that also has this property, and whose prior is concentrated on (a countable subset of) C.

7.1.5. Imitation and Inverse Reinforcement Learning

Score-based Inverse Reinforcement Learning, [29]

This paper reports theoretical and empirical results obtained for the score-based Inverse Reinforcement Learning (IRL) algorithm. It relies on a non-standard setting for IRL consisting of learning a reward from a set of globally scored trajec-tories. This allows using any type of policy (optimal or not) to generate trajectories without prior knowledge during data collection. This way, any existing database (like logs of systems in use) can be scored a posteriori by an expert and used to learn a reward function. Thanks to this reward function, it is shown that a near-optimal policy can be computed. Being related to least-square regression, the algorithm (called SBIRL) comes with theoretical guarantees that are proven in this paper. SBIRL is compared to standard IRL algorithms on synthetic data showing that annotations do help under conditions on the quality of the trajectories. It is also shown to be suitable for real-world applications such as the optimisation of a spoken dialogue system.

7.1.6. Stochastic Games

Blazing the trails before beating the path: Sample-efficient Monte-Carlo planning, [37]

You are a robot and you live in a Markov decision process (MDP) with a finite or an infinite number of transitions from state-action to next states. You got brains and so you plan before you act. Luckily, your roboparents equipped you with a generative model to do some Monte-Carlo planning. The world is waiting for you and you have no time to waste. You want your planning to be efficient. Sample-efficient. Indeed, you want to exploit the possible structure of the MDP by exploring only a subset of states reachable by following near-optimal policies. You want guarantees on sample complexity that depend on a measure of the quantity of near-optimal states. You want something, that is an extension of Monte-Carlo sampling (for estimating an expectation) to problems that alternate maximization (over actions) and expectation (over next states). But you do not want to StOP with exponential running time, you want something simple to implement and computationally efficient. You want it all and you want it now. You want TrailBlazer.

Maximin Action Identification: A New Bandit Framework for Games, [34]

We study an original problem of pure exploration in a strategic bandit model motivated by Monte Carlo Tree Search. It consists in identifying the best action in a game, when the player may sample random outcomes of sequentially chosen pairs of actions. We propose two strategies for the fixed-confidence setting: Maximin-LUCB, based on lower-and upper-confidence bounds; and Maximin-Racing, which operates by successively eliminating the sub-optimal actions. We discuss the sample complexity of both methods and compare their performance empirically. We sketch a lower bound analysis, and possible connections to an optimal algorithm.

7.2. Statistical analysis of time series

7.2.1. Change Point Analysis

Nonparametric multiple change point estimation in highly dependent time series, [18] Given a heterogeneous time-series sample, the objective is to find points in time, called change points, where the probability distribution generating the data has changed. The data are assumed to have been generated by arbitrary unknown stationary ergodic distributions. No modelling, independence or mixing assumptions are made. A novel, computationally efficient, nonparametric method is proposed, and is shown to be asymptotically consistent in this general framework. The theoretical results are complemented with experimental evaluations.

7.2.2. Clustering Time Series, Online and Offline

Consistent Algorithms for Clustering Time Series, [19]

The problem of clustering is considered for the case where every point is a time series. The time series are either given in one batch (offline setting), or they are allowed to grow with time and new time series can be added along the way (online setting). We propose a natural notion of consistency for this problem, and show that there are simple, com-putationally efficient algorithms that are asymptotically consistent under extremely weak assumptions on the distributions that generate the data. The notion of consistency is as follows. A clustering algorithm is called consistent if it places two time series into the same cluster if and only if the distribution that generates them is the same. In the considered framework the time series are allowed to be highly dependent, and the dependence can have arbitrary form. If the number of clusters is known, the only assumption we make is that the (marginal) distribution of each time series is stationary ergodic. No parametric, memory or mixing assumptions are made. When the number of clusters is unknown, stronger assumptions are provably necessary, but it is still possible to devise nonparametric algorithms that are consistent under very general conditions. The theoretical findings of this work are illustrated with experiments on both synthetic and real data.

7.2.3. Automata Learning

PAC learning of Probabilistic Automaton based on the Method of Moments, [36]

Probabilitic Finite Automata (PFA) are gener-ative graphical models that define distributions with latent variables over finite sequences of symbols, a.k.a. stochastic languages. Traditionally , unsupervised learning of PFA is performed through algorithms that iteratively improves the likelihood like the Expectation-Maximization (EM) algorithm. Recently, learning algorithms based on the so-called Method of Moments (MoM) have been proposed as a much faster alternative that comes with PAC-style guarantees. However, these algorithms do not ensure the learnt automata to model a proper distribution , limiting their applicability and preventing them to serve as an initialization to iterative algorithms. In this paper, we propose a new MoM-based algorithm with PAC-style guarantees that learns automata defining proper distributions. We assess its performances on synthetic problems from the PAutomaC challenge and real datasets extracted from Wikipedia against previous MoM-based algorithms and EM algorithm.

7.2.4. Online Kernel and Graph-Based Methods

Analysis of Nyström method with sequential ridge leverage score sampling, [26]

Large-scale kernel ridge regression (KRR) is limited by the need to store a large kernel matrix Kt. To avoid storing the entire matrix Kt, Nystro¨m methods subsample a subset of columns of the kernel matrix, and efficiently find an approximate KRR solution on the reconstructed Kt . The chosen subsampling distribution in turn affects the statistical and computational tradeoffs. For KRR problems, [15, 1] show that a sampling distribution proportional to the ridge leverage scores (RLSs) provides strong reconstruction guarantees for Kt. While exact RLSs are as difficult to compute as a KRR solution, we may be able to approximate them well enough. In this paper, we study KRR problems in a sequential setting and introduce the INK-ESTIMATE algorithm, that incrementally computes the RLSs estimates. INK-ESTIMATE maintains a small sketch of Kt, that at each step is used to compute an intermediate estimate of the RLSs. First, our sketch update does not require access to previously seen columns, and therefore a single pass over the kernel matrix is sufficient. Second, the algorithm requires a fixed, small space budget to run dependent only on the effective dimension of the kernel matrix. Finally, our sketch provides strong approximation guarantees on the distance $||Kt - Kt||^2$

, and on the statistical risk of the approximate KRR solution at any time, because all our guarantees hold at any intermediate step.

7.3. Statistical Learning and Bayesian Analysis

7.3.1. Non-parametric methods for Function Approximation

Pliable rejection sampling, [30]

Rejection sampling is a technique for sampling from difficult distributions. However, its use is limited due to a high rejection rate. Common adaptive rejection sampling methods either work only for very specific distributions or without performance guarantees. In this paper, we present pliable rejection sampling (PRS), a new approach to rejection sampling, where we learn the sampling proposal using a kernel estimator. Since our method builds on rejection sampling, the samples obtained are with high probability i.i.d. and distributed according to f. Moreover, PRS comes with a guarantee on the number of accepted samples.

7.3.2. Non-parametric methods for functional supervised learning

Operator-valued Kernels for Learning from Functional Response Data, [16]

In this paper we consider the problems of supervised classification and regression in the case where attributes and labels are functions: a data is represented by a set of functions, and the label is also a function. We focus on the use of reproducing kernel Hilbert space theory to learn from such functional data. Basic concepts and properties of kernel-based learning are extended to include the estimation of function-valued functions. In this setting, the representer theorem is restated, a set of rigorously defined infinite-dimensional operator-valued kernels that can be valuably applied when the data are functions is described, and a learning algorithm for nonlinear functional data analysis is introduced. The methodology is illustrated through speech and audio signal processing experiments.

7.3.3. Differential privacy

On the Differential Privacy of Bayesian Inference, [51]

We study how to communicate findings of Bayesian inference to third parties, while preserving the strong guarantee of differential privacy. Our main contributions are four different algorithms for private Bayesian inference on proba-bilistic graphical models. These include two mechanisms for adding noise to the Bayesian updates, either directly to the posterior parameters, or to their Fourier transform so as to preserve update consistency. We also utilise a recently introduced posterior sampling mechanism, for which we prove bounds for the specific but general case of discrete Bayesian networks; and we introduce a maximum-a-posteriori private mechanism. Our analysis includes utility and privacy bounds, with a novel focus on the influence of graph structure on privacy. Worked examples and experiments with Bayesian naïve Bayes and Bayesian linear regression illustrate the application of our mechanisms.

Algorithms for Differentially Private Multi-Armed Bandits, [50]

We present differentially private algorithms for the stochastic Multi-Armed Bandit (MAB) problem. This is a problem for applications such as adaptive clinical trials, experiment design, and user-targeted advertising where private information is connected to individual rewards. Our major contribution is to show that there exist (ϵ, δ) differentially private variants of Upper Confidence Bound algorithms which have optimal regret, $O(\epsilon^{-1} + \log T)$. This is a significant improvement over previous results, which only achieve poly-log regret $O(\epsilon^{-2} \log^2 T)$, because of our use of a novel interval-based mechanism. We also substantially improve the bounds of previous family of algorithms which use a continual release mechanism. Experiments clearly validate our theoretical bounds.

7.4. Applications

7.4.1. Spoken Dialogue Systems

Compact and Interpretable Dialogue State Representation with Genetic Sparse Distributed Memory, [28] t User satisfaction is often considered as the objective that should be achieved by spoken dialogue systems. This is why, the reward function of Spoken Dialogue Systems (SDS) trained by Reinforcement Learning (RL) is often designed to reflect user satisfaction. To do so, the state space representation should be based on features capturing user satisfaction characteristics such as the mean speech recognition confidence score for instance. On the other hand, for deployment in industrial systems, there is a need for state representations that are understandable by system engineers. In this paper, we propose to represent the state space using a Genetic Sparse Distributed Memory. This is a state aggregation method computing state prototypes which are selected so as to lead to the best linear representation of the value function in RL. To do so, previous work on Genetic Sparse Distributed Memory for classification is adapted to the Reinforcement Learning task and a new way of building the prototypes is proposed. The approach is tested on a corpus of dialogues collected with an appointment scheduling system. The results are compared to a grid-based linear parametrisation. It is shown that learning is accelerated and made more memory efficient. It is also shown that the framework is calable in that it is possible to include many dialogue features in the representation, interpret the resulting policy and identify the most important dialogue features.

A Stochastic Model for Computer-Aided Human-Human Dialogue, [24]

In this paper we introduce a novel model for computer-aided human-human dialogue. In this context, the computer aims at improving the outcome of a human-human task-oriented dialogue by intervening during the course of the interaction. While dialogue state and topic tracking in human-human dialogue have already been studied, few work has been devoted to the sequential part of the problem, where the impact of the system's actions on the future of the conversation is taken into account. This paper addresses this issue by first modelling human-human dialogue as a Markov Reward Process. The task of purposely taking part into the conversation is then optimised within the Linearly Solvable Markov Decision Process framework. Utterances of the Conversational Agent are seen as perturbations in this process, which aim at satisfying the user's long-term goals while keeping the conversation natural. Finally, results obtained by simulation suggest that such an approach is suitable for computer-aided human-human dialogue and is a first step towards three-party dialogue.

Learning Dialogue Dynamics with the Method of Moments, [25]

In this paper, we introduce a novel framework to encode the dynamics of dialogues into a probabilistic graphical model. Traditionally, Hidden Markov Models (HMMs) would be used to address this problem, involving a first step of hand-crafting to build a dialogue model (e.g. defining potential hidden states) followed by applying expectation-maximisation (EM) algorithms to refine it. Recently, an alternative class of algorithms based on the Method of Moments (MoM) has proven successful in avoiding issues of the EM-like algorithms such as convergence towards local optima, tractability issues, initialization issues or the lack of theoretical guarantees. In this work, we show that dialogues may be modeled by SP-RFA, a class of graphical models efficiently learnable within the MoM and directly usable in planning algorithms (such as reinforcement learning). Experiments are led on the Ubuntu corpus and dialogues are considered as sequences of dialogue acts, represented by their Latent Dirichlet Allocation (LDA) and Latent Semantic Analysis (LSA). We show that a MoM-based algorithm can learn a compact model of sequences of such acts.

7.4.2. Software development

Mutation-Based Graph Inference for Fault Localization, [45]

We present a new fault localization algorithm, called Vautrin, built on an approximation of causality based on call graphs. The approximation of causality is done using software mutants. The key idea is that if a mutant is killed by a test, certain call graph edges within a path between the mutation point and the failing test are likely causal. We evaluate our approach on the fault localization benchmark by Steimann et al. totaling 5,836 faults. The causal graphs are extracted from 88,732 nodes connected by 119,531 edges. Vautrin improves the fault localization effectiveness for all subjects of the benchmark. Considering the wasted effort at the method level, a classical fault localization evaluation metric, the improvement ranges from 3

A Large-scale Study of Call Graph-based Impact Prediction using Mutation Testing, [21] In software engineering, impact analysis consists in predicting the software elements (e.g. modules, classes, methods) potentially impacted by a change in the source code. Impact analysis is required to optimize the testing effort. In this paper, we propose a framework to predict error propagation. Based on 10 open-source Java projects and 5 classical mutation operators, we create 17000 mutants and study how the error they introduce propagates. This framework enables us to analyze impact prediction based on four types of call graph. Our results show that the sophistication indeed increases completeness of impact prediction. However, and surprisingly to us, the most basic call graph gives the highest trade-off between precision and recall for impact prediction.

A Learning Algorithm for Change Impact Prediction, [44]

Change impact analysis (CIA) consists in predicting the impact of a code change in a software application. In this paper, the artifacts that are considered for CIA are methods of object-oriented software; the change under study is a change in the code of the method, the impact is the test methods that fail because of the change that has been performed. We propose LCIP, a learning algorithm that learns from past impacts to predict future impacts. To evaluate LCIP, we consider Java software applications that are strongly tested. We simulate 6000 changes and their actual impact through code mutations, as done in mutation testing. We find that LCIP can predict the impact with a precision of 74

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6. New Results

6.1. Regularized Nonlinear Acceleration

In [34], describe a convergence acceleration technique for generic optimization problems. Our scheme computes estimates of the optimum from a nonlinear average of the iterates produced by any optimization method. The weights in this average are computed via a simple linear system, whose solution can be updated online. This acceleration scheme runs in parallel to the base algorithm, providing improved estimates of the solution on the fly, while the original optimization method is running. Numerical experiments are detailed on classical classification problems.

6.2. Harder, Better, Faster, Stronger Convergence Rates for Least-Squares Regression

In [20], we consider the optimization of a quadratic objective function whose gradients are only accessible through a stochastic oracle that returns the gradient at any given point plus a zero-mean finite variance random error. We present the first algorithm that achieves jointly the optimal prediction error rates for least-squares regression, both in terms of forgetting of initial conditions in $O(1/n^2)$, and in terms of dependence on the noise and dimension d of the problem, as $O(d/n)$. Our new algorithm is based on averaged accelerated regularized gradient descent, and may also be analyzed through finer assumptions on initial conditions and the Hessian matrix, leading to dimension-free quantities that may still be small while the " optimal " terms above are large. In order to characterize the tightness of these new bounds, we consider an application to non-parametric regression and use the known lower bounds on the statistical performance (without computational limits), which happen to match our bounds obtained from a single pass on the data and thus show optimality of our algorithm in a wide variety of particular trade-offs between bias and variance.

6.3. Stochastic Variance Reduction Methods for Saddle-Point Problems

In [12], we consider convex-concave saddle-point problems where the objective functions may be split in many components, and extend recent stochastic variance reduction methods (such as SVRG or SAGA) to provide the first large-scale linearly convergent algorithms for this class of problems which are common in machine learning. While the algorithmic extension is straightforward, it comes with challenges and opportunities: (a) the convex minimization analysis does not apply and we use the notion of monotone operators to prove convergence, showing in particular that the same algorithm applies to a larger class of problems, such as variational inequalities, (b) there are two notions of splits, in terms of functions, or in terms of partial derivatives, (c) the split does need to be done with convex-concave terms, (d) non-uniform sampling is key to an efficient algorithm, both in theory and practice, and (e) these incremental algorithms can be easily accelerated using a simple extension of the “catalyst” framework, leading to an algorithm which is always superior to accelerated batch algorithms.

6.4. Frank-Wolfe Algorithms for Saddle Point Problems

In [26], we extend the Frank-Wolfe (FW) optimization algorithm to solve constrained smooth convex-concave saddle point (SP) problems. Remarkably, the method only requires access to linear minimization oracles. Leveraging recent advances in FW optimization, we provide the first proof of convergence of a FW-type saddle point solver over polytopes, thereby partially answering a 30 year-old conjecture. We also survey other convergence results and highlight gaps in the theoretical underpinnings of FW-style algorithms. Motivating applications without known efficient alternatives are explored through structured predic- tion with combinatorial penalties as well as games over matching polytopes involving an exponential number of constraints.

6.5. Minding the Gaps for Block Frank-Wolfe Optimization of Structured SVM

In [10], we propose several improvements on the block-coordinate Frank-Wolfe (BCFW) algorithm from Lacoste-Julien et al. (2013) recently used to optimize the structured support vector machine (SSVM) objective in the context of structured prediction, though it has wider applications. The key intuition behind our improvements is that the estimates of block gaps maintained by BCFW reveal the block suboptimality that can be used as an adaptive criterion. First, we sample objects at each iteration of BCFW in an adaptive non-uniform way via gapbased sampling. Second, we incorporate pairwise and away-step variants of Frank-Wolfe into the block-coordinate setting. Third, we cache oracle calls with a cache-hit criterion based on the block gaps. Fourth, we provide the first method to compute an approximate regularization path for SSVM. Finally, we provide an exhaustive empirical evaluation of all our methods on four structured prediction datasets. The associated SOFTWARE is here: https://github.com/aosokin/gapBCFW

6.6. Asaga: Asynchronous Parallel Saga

In [29], we describe Asaga, an asynchronous parallel version of the incremental gradient algorithm Saga that enjoys fast linear convergence rates. We highlight a subtle but important technical issue present in a large fraction of the recent convergence rate proofs for asynchronous parallel optimization algorithms, and propose a simplification of the recently proposed "perturbed iterate" framework that resolves it. We thereby prove that Asaga can obtain a theoretical linear speedup on multi-core systems even without sparsity assumptions. We present results of an implementation on a 40-core architecture illustrating the practical speedup as well as the hardware overhead.

6.7. Convergence Rate of Frank-Wolfe for Non-Convex Objectives

In [28], we give a simple proof that the Frank-Wolfe algorithm obtains a stationary point at a rate of $O(1/\sqrt{t})$ on non-convex objectives with a Lipschitz continuous gradient. Our analysis is affine invariant and is the first, to the best of our knowledge, giving a similar rate to what was already proven for projected gradient methods (though on slightly different measures of stationarity).

6.8. Highly-Smooth Zero-th Order Online Optimization

The minimization of convex functions which are only available through partial and noisy infor- mation is a key methodological problem in many disciplines. In [3], we consider convex optimization with noisy zero-th order information, that is noisy function evaluations at any desired point. We focus on problems with high degrees of smoothness, such as logistic regression. We show that as opposed to gradient-based algorithms, high-order smoothness may be used to improve estimation rates, with a precise dependence of our upper-bounds on the degree of smoothness. In particular, we show that for infinitely differentiable functions, we recover the same dependence on sample size as gradient-based algorithms, with an extra dimension-dependent factor. This is done for both convex and strongly-convex functions, with finite horizon and anytime algorithms. Finally, we also recover similar results in the online optimization setting.

6.9. Slice Inverse Regression with Score Functions

Non-linear regression and related problems such as non-linear classification are core important tasks in machine learning and statistics. We consider the problem of dimension reduction in non-linear regression, which is often formulated as a non-convex optimization problem.

- We propose score function extensions to sliced inverse regression problems [38], [39], both for the first-order and second-order score functions, which provably improve estimation in the population case over the non-sliced versions; we study finite sample estimators and study their consistency given the exact score functions.
- We propose also to learn the score function as well (using score matching technique [37]) in two steps, i.e., first learning the score function and then learning the effective dimension reduction space, or directly, by solving a convex optimization problem regularized by the nuclear norm.

6.10. Inference and learning for log-supermodular distributions

In [11], we consider log-supermodular models on binary variables, which are probabilistic models with negative log-densities which are submodular. These models provide probabilistic interpretations of common combinatorial optimization tasks such as image segmentation. We make the following contributions:

- We review existing variational bounds for the log-partition function and show that the bound of T. Hazan and T. Jaakkola (On the Partition Function and Random Maximum A-Posteriori Perturbations, Proc. ICML, 2012), based on "perturb-and-MAP" ideas, formally dominates the bounds proposed by J. Djolonga and A. Krause (From MAP to Marginals: Variational Inference in Bayesian Submodular Models, Adv. NIPS, 2014).
- We show that for parameter learning via maximum likelihood the existing bound of J. Djolonga and A. Krause typically leads to a degenerate solution while the one based on "perturb-and-MAP" ideas and logistic samples does not.
- Given that the bound based on "perturb-and-MAP" ideas is an expectation (over our own randomization), we propose to use a stochastic subgradient technique to maximize the lower-bound on the log-likelihood, which can also be extended to conditional maximum likelihood.
- We illustrate our new results on a set of experiments in binary image denoising, where we highlight the flexibility of a probabilistic model for learning with missing data.

6.11. Beyond CCA: Moment Matching for Multi-View Models

In [31], we introduce three novel semi-parametric extensions of probabilistic canonical correlation analysis with identifiability guarantees. We consider moment matching techniques for estimation in these models. For that, by drawing explicit links between the new models and a discrete version of independent component analysis (DICA), we first extend the DICA cumulant tensors to the new discrete version of CCA. By further using a close connection with independent component analysis, we introduce generalized covariance matrices, which can replace the cumulant tensors in the moment matching framework, and, therefore, improve sample complexity and simplify derivations and algorithms significantly. As the tensor power method or orthogonal joint diagonalization are not applicable in the new setting, we use non-orthogonal joint diagonalization techniques for matching the cumulants. We demonstrate performance of the proposed models and estimation techniques on experiments with both synthetic and real datasets.

6.12. PAC-Bayesian Theory Meets Bayesian Inference

In [6], we exhibit a strong link between frequentist PAC-Bayesian bounds and the Bayesian marginal likelihood. That is, for the negative log-likelihood loss function, we show that the minimization of PAC-Bayesian generalization bounds maximizes the Bayesian marginal likelihood. This provides an alternative explanation to the Bayesian Occam's razor criteria, under the assumption that the data is generated by an *i.i.d.* distribution. Moreover, as the negative log-likelihood is an unbounded loss function, we motivate and propose a PAC-Bayesian theorem tailored for the sub-gamma loss family, and we show that our approach is sound on classical Bayesian linear regression tasks.

6.13. A New PAC-Bayesian Perspective on Domain Adaptation

In [7], we study the issue of PAC-Bayesian domain adaptation: We want to learn, from a source domain, a majority vote model dedicated to a target one. Our theoretical contribution brings a new perspective by deriving an upper-bound on the target risk where the distributions' divergence— expressed as a ratio—controls the trade-off between a source error measure and the target voters' disagreement. Our bound suggests that one has to focus on regions where the source data is informative. From this result, we derive a PAC-Bayesian generalization bound, and specialize it to linear classifiers. Then, we infer a learning algorithm and perform experiments on real data.

6.14. PAC-Bayesian Bounds based on the Rényi Divergence

In [13], we propose a simplified proof process for PAC-Bayesian generalization bounds, that allows to divide the proof in four successive inequalities, easing the "customization" of PAC-Bayesian theorems. We also propose a family of PAC-Bayesian bounds based on the Rényi divergence between the prior and posterior distributions, whereas most PAC-Bayesian bounds are based on the Kullback-Leibler divergence. Finally, we present an empirical evaluation of the tightness of each inequality of the simplified proof, for both the classical PAC-Bayesian bounds and those based on the Rényi divergence.

6.15. PAC-Bayesian theorems for multiview learning

In [27], we tackle the issue of multiview learning which aims to take advantages of multiple representations/views of the data. In this context, many machine learning algorithms exist. However, the majority of the theoretical studies focus on learning with exactly two representations. In this paper, we propose a general PAC-Bayesian theory for multiview learning with more than two views. We focus our study to binary classification models that take the form of a majority vote. We derive PAC-Bayesian generalization bounds allowing to consider different relations between empirical and true risks by taking into account a notion of diversity of the voters and views, and that can be naturally extended to semi-supervised learning.

6.16. A spectral algorithm for fast de novo layout of uncorrected long nanopore reads

Seriation is an optimization problem that seeks to reconstruct an ordering between n variables from pairwise similarity information. It can be formulated as a combinatorial problem over permutations and several algorithms have been derived from relaxations of this problem. We make the link between the seriation framework and the task of de novo genome assembly, which consists of reconstructing a whole DNA sequence from small pieces of it that are oversampled so as to cover the full genome. To achieve this task, one has to find the layout of small pieces of DNA sequences (reads). This layout step can be cast as a seriation problem. We show that a spectral algorithm for seriation can be efficiently applied to a genome assembly scheme.

New long read sequencers promise to transform sequencing and genome assembly by producing reads tens of kilobases long. However their high error rate significantly complicates assembly and requires expensive correction steps to layout the reads using standard assembly engines.

We present an original and efficient spectral algorithm to layout the uncorrected nanopore reads, and its seamless integration into a straightforward overlap/layout/consensus (OLC) assembly scheme. The method is shown to assemble Oxford Nanopore reads from several bacterial genomes into good quality ($\sim 99\%$ identity to the reference) genome-sized contigs, while yielding more fragmented assemblies from a *Sacharomyces cerevisiae* reference strain. See software in https://github.com/antrec/spectrassembler.

6.17. Using Deep Learning and Generative Adversarial Networks to Study Large Scale GFP Screens

Fluorescent imaging of GFP tagged proteins is one of the most widely used techniques to view the dynamics of proteins in live cells. By combining it with different perturbations such as RNAi or drug treatments we can understand how cells regulate complex processes such as mitosis or the cell cycle.

However, GFP imaging has certain limitations. There are only a limited number of different fluorescent proteins available, making imaging multiple proteins at the same time very challenging and expensive. Finally, analyzing complex screens can be very challenging: it's not always obvious a-priori what kind of features will predict the phenotypes we are interested in.

We discuss a new approach to studying large scale GFP screens using deep convolutional networks. We show that by using convolutional neural networks, we can greatly outperform traditional feature based approaches at different kind of prediction tasks. The networks learn flexible representations, which are suitable for multiple tasks, such as predicting the localization of Tea1 in fission yeast cells (blue signal, shown in image) in cells where only other proteins are tagged.

We then show that we can use generative adversarial neural networks to learn highly compact latent representations. Those latent representations can then be used to generate new realistic images, allowing us to simulate new phenotypes, and to predict the outcome of new perturbations (joint work between Federico Vaggi, Anton Osokin, Theophile Dalens).

6.18. SymPy: Symbolic computing in Python

SymPy is an open source computer algebra system written in pure Python. It is built with a focus on extensibility and ease of use, through both interactive and programmatic applications. These characteristics have led SymPy to become the standard symbolic library for the scientific Python ecosystem. This paper [30] presents the architecture of SymPy, a description of its features, and a discussion of select domain specific submodules. The supplementary materials provide additional examples and further outline details of the architecture and features of SymPy. As for the software, I am one of the main authors of the lightning machine learning library, that you can include if you want.

6.19. Robust Discriminative Clustering with Sparse Regularizers

Clustering high-dimensional data often requires some form of dimensionality reduction, where clustered variables are separated from "noise-looking" variables. In [24], we cast this problem as finding a low-dimensional projection of the data which is well-clustered. This yields a one-dimensional projection in the simplest situation with two clusters, and extends naturally to a multi-label scenario for more than two clusters. In this paper, (a) we first show that this joint clustering and dimension reduction formulation is equivalent to previously proposed discriminative clustering frameworks, thus leading to convex relaxations of the problem, (b) we propose a novel sparse extension, which is still cast as a convex relaxation and allows estimation in higher dimensions, (c) we propose a natural extension for the multi-label scenario, (d) we provide a new theoretical analysis of the performance of these formulations with a simple probabilistic model, leading to scalings over the form $d = O(\sqrt{n})$ for the affine invariant case and $d = O(n)$ for the sparse case, where n is the number of examples and d the ambient dimension, and finally, (e) we propose an efficient iterative algorithm with running-time complexity proportional to $O(nd^2)$, improving on earlier algorithms which had quadratic complexity in the number of examples.

6.20. Optimal Rates of Statistical Seriation

Given a matrix the seriation problem consists in permuting its rows in such way that all its columns have the same shape, for example, they are monotone increasing. In [23], we propose a statistical approach to this problem where the matrix of interest is observed with noise and study the corresponding minimax rate of estimation of the matrices. Specifically, when the columns are either unimodal or monotone, we show that the least squares estimator is optimal up to logarithmic factors and adapts to matrices with a certain natural structure. Finally, we propose a computationally efficient estimator in the monotonic case and study its performance both theoretically and experimentally. Our work is at the intersection of shape constrained estimation and recent work that involves permutation learning, such as graph denoising and ranking.

6.21. Breaking Sticks and Ambiguities with Adaptive Skip-gram

Recently proposed Skip-gram model is a powerful method for learning high-dimensional word representations that capture rich semantic relationships between words. However, Skip-gram as well as most prior work on learning word representations does not take into account word ambiguity and maintain only single representation per word. Although a number of Skip-gram modifications were proposed to overcome this limitation and learn multi-prototype word representations, they either require a known number of word meanings or learn them using greedy heuristic approaches. In [4], we propose the Adaptive Skip-gram model which is a nonparametric Bayesian extension of Skip-gram capable to automatically learn the required number of representations for all words at desired semantic resolution. We derive efficient online variational learning algorithm for the model and empirically demonstrate its efficiency on word-sense induction task.

6.22. Deep Part-Based Generative Shape Model with Latent Variables

The Shape Boltzmann Machine (SBM) and its multilabel version MSBM [5] have been recently introduced as deep generative models that capture the variations of an object shape. While being more flexible MSBM requires datasets with labeled parts of the objects for training. In [8], we present an algorithm for training MSBM using binary masks of objects and the seeds which approximately correspond to the locations of objects parts. The latter can be obtained from part-based detectors in an unsupervised manner. We derive a latent variable model and an EM-like training procedure for adjusting the weights of MSBM using a deep learning framework. We show that the model trained by our method outperforms SBM in the tasks related to binary shapes and is very close to the original MSBM in terms of quality of multilabel shapes.

6.23. Unsupervised Learning from Narrated Instruction Videos

In [2], we address the problem of automatically learning the main steps to complete a certain task, such as changing a car tire, from a set of narrated instruction videos. The contributions of this paper are three-fold. First, we develop a new unsupervised learning approach that takes advantage of the complementary nature of the input video and the associated narration. The method solves two clustering problems, one in text and one in video, applied one after each other and linked by joint constraints to obtain a single coherent sequence of steps in both modalities. Second, we collect and annotate a new challenging dataset of real-world instruction videos from the Internet. The dataset contains about 800,000 frames for five different tasks that include complex interactions between people and objects, and are captured in a variety of indoor and outdoor settings. Third, we experimentally demonstrate that the proposed method can automatically discover, in an unsupervised manner, the main steps to achieve the task and locate the steps in the input videos. The associated SOFTWARE is here: https://github.com/jalayrac/instructionVideos

6.24. Stochastic Optimization for Large-scale Optimal Transport

Optimal transport (OT) defines a powerful framework to compare probability distributions in a geometrically faithful way. However, the practical impact of OT is still limited because of its computational burden. In [5], we propose a new class of stochastic optimization algorithms to cope with large-scale OT problems. These methods can handle arbitrary distributions (either discrete or continuous) as long as one is able to draw samples from them, which is the typical setup in high-dimensional learning problems. This alleviates the need to discretize these densities, while giving access to provably convergent methods that output the correct distance without discretization error. These algorithms rely on two main ideas: *(a)* the dual OT problem can be re-cast as the maximization of an expectation; *(b)* the entropic regularization of the primal OT problem yields a smooth dual optimization which can be addressed with algorithms that have a provably faster convergence. We instantiate these ideas in three different setups: *(i)* when comparing a discrete distribution to another, we show that incremental stochastic optimization schemes can beat Sinkhorn's algorithm, the current state-of-the-art finite dimensional OT solver; *(ii)* when comparing a discrete distribution to a continuous density, a semi-discrete reformulation of the dual program is amenable to averaged stochastic gradient descent, leading to better performance than approximately solving the problem by discretization ; *(iii)* when dealing with two continuous densities, we propose a stochastic gradient descent over a reproducing kernel Hilbert space (RKHS). This is currently the only known method to solve this problem, apart from computing OT on finite samples. We backup these claims on a set of discrete, semi-discrete and continuous benchmark problems.

6.25. Online but Accurate Inference for Latent Variable Models with Local Gibbs Sampling

We study parameter inference in large-scale latent variable models. We first propose a unified treatment of online inference for latent variable models from a non-canonical exponential family, and draw explicit links between several previously proposed frequentist or Bayesian methods. We then propose a novel inference method for the frequentist estimation of parameters, that adapts MCMC methods to online inference of latent variable models with the proper use of local Gibbs sampling. Then, for latent Dirichlet allocation,we provide an extensive set of experiments and comparisons with existing work, where our new approach outperforms all previously proposed methods. In particular, using Gibbs sampling for latent variable inference is superior to variational inference in terms of test log-likelihoods. Moreover, Bayesian inference through variational methods perform poorly, sometimes leading to worse fits with latent variables of higher dimensionality.

In [22], we focus on methods that make a single pass over the data to estimate parameters. We make the following contributions:

1. We review and compare existing methods for online inference for latent variable models from a non-canonical exponential family, and draw explicit links between several previously proposed frequentist or Bayesian methods. Given the large number of existing methods, our unifying framework allows to understand differences and similarities between all of them.
2. We propose a novel inference method for the frequentist estimation of parameters, that adapts MCMC methods to online inference of latent variable models with the proper use of "local" Gibbs sampling. In our online scheme, we apply Gibbs sampling to the current observation, which is "local", as opposed to "global" batch schemes where Gibbs sampling is applied to the entire dataset.
3. After formulating LDA as a non-canonical exponential family, we provide an extensive set of experiments, where our new approach outperforms all previously proposed methods. In particular, using Gibbs sampling for latent variable inference is superior to variational inference in terms of test log-likelihoods. Moreover, Bayesian inference through variational methods perform poorly, sometimes leading to worse fits with latent variables of higher dimensionality.

6.26. Learning Determinantal Point Processes in Sublinear Time

In [21], we propose a new class of determinantal point processes (DPPs) which can be manipulated for inference and parameter learning in potentially sublinear time in the number of items. This class, based on a specific low-rank factorization of the marginal kernel, is particularly suited to a subclass of continuous DPPs and DPPs defined on exponentially many items. We apply this new class to modelling text documents as sampling a DPP of sentences, and propose a conditional maximum likelihood formulation to model topic proportions, which is made possible with no approximation for our class of DPPs. We present an application to document summarization with a DPP on 2^{500} items.

We make the following contributions:

- We propose a new class of determinantal point processes (DPPs) which is based on a particular low-rank factorization of the marginal kernel. Through the availability of a particular second-moment matrix, the complexity for inference and learning tasks is polynomial in the rank of the factorization and thus often sublinear in the total number of items (with exact likelihood computations).
- As shown in this work, these new DPPs are particularly suited to a subclass of continuous DPPs (infinite number of items), such as on $[0,1]^m$, and DPPs defined on the V-dimensional hypercube, which has 2^V elements.
- We propose a model of documents as sampling a DPP of sentences, and propose a conditional maximum likelihood formulation to model topic proportions. We present an application to document summarization with a DPP on 2^{500} items.

6.27. Decentralized Topic Modelling with Latent Dirichlet Allocation

Privacy preserving networks can be modelled as decentralized networks (e.g., sensors, connected objects, smartphones), where communication between nodes of the network is not controlled by a master or central node. For this type of networks, the main issue is to gather/learn global information on the network (e.g., by optimizing a global cost function) while keeping the (sensitive) information at each node. In this work, we focus on text information that agents do not want to share (e.g., text messages, emails, confidential reports). We use recent advances on decentralized optimization and topic models to infer topics from a graph with limited communication. We propose a method to adapt latent Dirichlet allocation (LDA) model to decentralized optimization and show on synthetic data that we still recover similar parameters and similar performance at each node than with stochastic methods accessing to the whole information in the graph.

In [14], we tackle the non-convex problem of topic modelling, where agents have sensitive text data at their disposal that they can not or do not want to share (e.g., text messages, emails, confidential reports). More precisely, we adapt the particular Latent Dirichlet Allocation (LDA) model to decentralized networks. We combine recent work of [22] on online inference for latent variable models, which adapts online EM with local Gibbs sampling in the case of intractable latent variable models (such as LDA) and recent advances on decentralized optimization.

TAO Project-Team

7. New Results

7.1. Optimal Decision Making under Uncertainty

The Tao UCT-SIG is working mainly on mathematical programming tools useful for power systems. In particular, we advocate a data science approach, in order to reduce the model error - which is much more critical than the optimization error, in most cases. Real data are the best way for handling uncertainties. Our main results in 2016 are as follows:

- **Noisy optimization** In the context of stochastic uncertainties, noisy optimization handles the model error by simulation-based optimization. Our results include:
  - It has been conjectured that gradient approximation by finite differences (hence, not a comparison-based method) is necessary for reaching such a simple regret of O(1/N). We answer this conjecture in the negative [32], providing a comparison-based algorithm as good as gradient methods, i.e. reaching O(1/N) - under the condition, however, that the noise is Gaussian.
  - The concept of Regret is widely used in the bandit literature for assessing the performance of an algorithm. The same concept is also used in the framework of optimization algorithms, sometimes under other names or without a specific name. Experimental results on the noisy sphere function show that the approximation of Simple Regret, termed Approximate Simple Regret, used in some optimization testbeds, fails to estimate the Simple Regret convergence rate, and propose a new approximation of Simple Regret, the Robust Simple Regret [22].
- **Capacity Expansion Planning** The optimization of capacities in large scale power systems is a stochastic problem, because the need for storage and connections (i.e. exchange capacities) varies a lot from one week/season to another. It is usually tackled through sample average approximation, i.e. assuming that the system which is optimal on average over the last 40 years (corrected for climate change) is also approximately optimal in general. However, in many cases, data are high-dimensional; the sample complexity, i.e. the amount of data necessary for a relevant optimization of capacities, increases linearly with the number of parameters and can be scarcely available at the relevant scale. This leads to an underestimation of capacities. We suggested the use of bias correction in capacity estimation, and investigated the importance of the bias phenomenon, and the efficiency of both standard and original bias correction tools [53].
- **Multi-armed bandits** We studied the problem of sequential decision making in the context of multi-armed bandits. We provided:
  - An algorithm to handle a non-stationary formulation of the stochastic multi-armed bandit where the rewards are not assumed to be identically distributed, that achieves both a competitive regret and sampling complexity against a best sequence of arms. See [61].
  - An algorithm to handle the task of recommending items (actions) to users sequentially interacting with a recommender system. Users are modeled as latent mixtures of C many representative user classes, where each class specifies a mean reward profile across actions. Both the user features (mixture distribution over classes) and the item features (mean reward vector per class) are unknown a priori. The user identity is the only contextual information available to the learner while interacting. This induces a low-rank structure on the matrix of expected rewards from recommending item a to user b. The problem reduces to the well-known linear bandit when either user-or item-side features are perfectly known. In the setting where each user, with its stochastically sampled taste profile, interacts only for a small number of sessions, we develop a bandit algorithm for the two-sided uncertainty. It combines the Robust Tensor Power Method with the OFUL linear bandit algorithm. We provide the first rigorous regret analysis of this combination. See [63].

- **Confidence intervals for streaming data** We consider, in a generic streaming regression setting, the problem of building a confidence interval (and distribution) on the next observation based on past observed data. The observations may have arbitrary dependency on the past observations and come from some external filtering process making the number of observations itself a random stopping time. In this challenging context, we provide confidence intervals based on self-normalized vector-valued martingale techniques, applied to the estimation of the mean and of the variance. See [69].
- **Forecasting tool for Hydraulic networks** We studied a problem of prediction in the context of the monitoring of an hydraulic network by the French company Prolog-ingenierie. The problem is to predict the value of some specific sensor in the next thirty minutes from the activity of the network (values of all other sensors) in the recent past. We designed a simple tool for that purpose, based on a random forests. The tool has been tested on data generated from the activity recorded on the Parisian hydraulic network in 2010, 2011 and 2013.

7.2. Continuous Optimization

- **Markov Chain Analysis of Evolution Strategies** The theory of Markov chains with discrete time and continuous state space turns out to be very useful to analyze the convergence of adaptive evolution strategies, including simplified versions of the state-of-the art CMA-ES. Exploiting invariance properties of the objective function and of a wide variety of comparison-based optimisation algorithms, we have developed a general methodology to prove global linear convergence [4]. The constructed Markov chains also show the connection between comparison-based adaptive stochastic algorithms and Markov chain Monte Carlo algorithms. Furthermore, we have continued to work on new theoretical tools that exploit deterministic control models to prove the irreducibility and T-chain property of general Markov chains. These tools promise to trivialise some stability proofs of the Markov chains we are interested in to analyse.
- **Large-scale Optimisation Algorithms** We have been working on (improved) variants of CMA-ES with more favorable scaling properties with the dimension. While computing and using the natural gradient in appropriate subspaces turned out to be considerably more difficult than expected, we explored variants that restrict the covariance via projection, so-called VkD-CMA-ES [21]. We derived a computationally efficient way to update the restricted covariance matrix, where the richness of the model is controlled by the integer parameter k. This parameter provides a smooth transition between the case where only diagonal elements are subject to changes and changes of the full covariance matrix. In the latter case, the update is equivalent with the original CMA-ES. In order to get rid of the control parameter we propose an adaptation of k which turns out to be surprisingly efficient [20].
- **Analysis of Lagrangian based Constraints Handling in Evolution Strategies** We have addressed the question of linear convergence of evolution strategies on constrained optimisation problems with one linear constraint. Based on previous works, we consider an adaptive augmented Lagrangian approach for the simple (1+1)-ES [23] and for the CMA-ES [24]. By design both algorithms derive from a framework with an underlying homogenous Markov chain which paves the way to prove linear convergence on a comparatively large class of functions. For the time being, stability of the Markov chain, associated with linear convergence, has been shown empirically on convex-quadratic and ill-conditioned functions.
- **Benchmarking of continuous optimizers** We have been pursuing our efforts towards improving the standards in benchmarking of continuous optimisers [65], [66], [64]. Three new testbeds have been developed and implemented. (i) A bi-objective testbed [74] where also a corresponding performance assessment procedure has been advised [62]. In this context, a new version of MO-CMA-ES has been developed and benchmarked [44] on this testbed. (ii) A large-scale testbed, as a straight forward extension of the standard tested. The extension is based on a general methodology we have developed to construct non-trivial but scalable test functions [19]. (iii) a constrained testbed (unpublished).

7.3. Data Science

- **High Energy Physics** The focus of the period has been to expand the collaboration with the High Energy Physics experiments started with the success of the 2014 HiggsML challenge [18] to new issues. The subject of V. Estrade Phd is to advance domain adaptation methods in the specific context of uncertainty quantification and calibration. So far, transfer learning has been addressed only with classical, additive and differentiable objective functions as performance criteria. However, learning to discover, exemplified by HEP, relies on more global and difficult criteria, related to the Area Under Roc Curve (AUC) and Neymann-Pearson learning. CERN funds another PhD (A. Pol), on anomaly detection. Another promising theme has emerged with the ongoing organization of a Tracking Challenge (TrackML) [56], [72], which focuses on extreme scaling of ML image processing.
- **Personal Semantics** Our algorithm for inducing a taxonomy from a set of domain terms, that was placed first in the international Taxonomy Induction task, part of the SemEval 2015 conference in Denver, has been improved by the development of a robust technique for discovering the domain vocabulary for a new topic using a directed crawler we created. We have created hundreds of taxonomy for personal themes (hobbies, illnesses) that can be integrated into our Personal Semantics platform PTraces, and have deployed and evaluated the taxonomies. We also have introduced newer machine learning methods, such as Latent Dirichlet Allocation, for better recognition of domain vocabularies [55], [71].
- **Distributed system observation** The work on distributed system automated analaysis and description has been persued thru the continued development of the GAMA multi-agent framework https://github.com/gama-platform/gama/wiki. The simulation framework has been applied to the study of a new protocol for MOOC management [6]. Philippe Caillou is associated to the young researcher ANR ACTEUR, coordinated by Patrick Taillandier (IDEES, Rouen university). With this project, the BDI cognitive agent model has been improved both in term of flexibility and ease of use for the non expert modeler [50].
- **Computational social sciences** Thomas Schmitt's PhD focuses on the matching of job offers and applicant CVs. An informal collaboration with the Qapa agency (FUI proposal underway) gave us access to the 2012-2016 logs of their activity (CVs, job announcements and application clicks). This wealth of data delivered some unexpected findings, e.g., as to the differences between people's practice (the clicks) and their say (the documents). In [49], with Philippe Caillou and Michèle Sebag, a deep NN system MAJORE (MAtching JObs and REsumes) was proposed, trained to match the metric properties extracted from the collaborative filtering matrix, and address the cold start problem. A further research perspective, in collaboration with J.-P. Nadal from EHESS, is to build an observatory of the job demand dynamics.

  The Cartolabe project, started in Feb. 2016 (F. Louistisserand's engineer stint), applies machine learning techniques to build an interpretable representation from vast amounts of scientific articles. The goal is to use raw textual data, and the results of the pre-processing chain achieved by ANHALYTICS, to define a topology on authors, scientific themes, and teams, and enforce its 2D projection in a semantically admissible way. The collaboration with AVIZ is key to enable the scalable and navigable exploitation of this map. The perspective for 2017 is to build a visual interrogation of the map (locating all author names relevant to a given request) and to display the temporal evolution of the research activities.

  Amiqap studies the relation between quality of life at work and company performance, using both survey data on individual workers (collected by DARES, the statistical service of the French Ministry of labor, in 2013) and administrative data on companies provided by SECAFI, a union body. The study is run by a team within TAO (Philippe Caillou, Isabelle Guyon, Michèle Sebag and Paola Tubaro, plus post-doctoral researcher Olivier Goudet and intern Diviyan Kalainathan) in collaboration with Mines ParisTech social science and economics (SES) department, the RITM economics research center (Univ. Paris Sud) and the think-tank La Fabrique de l'Industrie. In its first stage, the exploratory analysis delivered some unexpected results, e.g. as to the existence of a "industry worker cluster", or the non-monotonous relationship between autonomy, salary and subjective satisfaction. A summary of these findings has been released online on the website of La

Fabrique de l'Industrie, as a complement to their book on the same topic (published in October 2016). The exploratory analysis of the SECAFI data (yet unpublished) complements the above and shows how workers' satisfaction correlates with companies' financial and social performance indicators, though with marked differences across industries. The key question regards the nature of this relationship: cause, effect or due to a confounder feature (the industrial sector). Further research (Diviyan Kalainathan's PhD, O. Goudet post-doc) will focus on the use and extension of causal modelling algorithms on this issue; these perspectives attract quite some interest from the ministry (DARES) and big industrial players, willing to assess the relevance of their HR policies.

7.4. Designing criteria

- **Algorithm selection and configuration** Two PhD theses are related to the former *Crossing the Chasm* SIG: Nacim Belkhir (CIFRE PhD with Thalès) is working on Per Instance Algorithm Configuration (PIAC) in the context of continuous optimization. He has worked on the use of surrogate models for feature computation in case of expensive objective functions [31] and has validated his work with Differential Evolution applied to BBOB testnehc [30]. Defence planned for March 2017.

  François Gonard's PhD is dedicated to optimization algorithm selection. The original application domain was that of expensive car industry simulations (within the IRT-ROM project). The lack of real test cases made him investigate some combinatorial optimization setting, for which there exist public datasets. François obtained a "Honorable mention from the jury" for his submission to the ICON Challenge (http://iconchallenge.insight-centre.org/), for its original approach coupling a pre-scheduler and an algorithm selector [39]. Defence is planned for November 2017.

  The work done during Mustafa Misir's post-doc stint (ERCIM 2013-2014), regarding the formalization and tackling of the algorithm selection problem in terms of a collaborative filtering problem, was finally published [15].

- **A statistical physics perspective** Our activity on probabilistic model design is progressively moving from static explicit interactions to dynamical ones and to latent variable models, taking inspiration from latent feature representations provided by deep learning techniques. Concerning explicit pairwise interactions models like in [14] initially motivated by traffic applications, a systematic treatment of loop corrections based on a minimal cycle basis [11] has led us to propose: (i) a fast and large scale generalized belief propagation method (GCBP) with more robust convergence properties than bare belief propagation (ii) an inverse approximate MRF with linear scaling of the computational time, compliant with GCBP (iii) a new sampling method based on extracting random sub-graph of tree-width 2 on which GCBP can provide exact marginals. More generally considering effect of problematic i.e. frustrated cycles open the possibility for new criteria in model design. In particular we have started to bridge this work with the analysis of multi-layer restricted Boltzmann machines (RBM). Remarkably these possess a planar dual representation and we are expecting the density of frustrated cycles nodes to play a key role when characterizing an RBM learned from structured data by contrast with purely random instances. Additionally we have identify some properties of the data themeselves that have to be taken into consideration when learning static [9] or dynamical [8] Ising models.

- **Artificial Immune Systems** Within the E-Lucid project with Thalès TERESIS, around anomaly detection in network trafic, a first approach has been developed using Artificial Immune System (AIS) and the concept of Voronoi representation. A first proof of concept was a poster at the GECCO conference [70], before a complete paper was published at the PPSN conference [46]. Note that this work on anomaly detection is on-going using Deep Learning. AIS are also the basis of Chaouki Boufenar's PhD work (visiting TAO from U. Oran, Algérie), with a first work on arabic characters recognition [5].

7.5. Deep Learning and Information Theory

- **Neural networks for computer vision** We continued working on the topic of large-scale image segmentation with multiple object detection. The application target is the analysis of high-resolution multispectral satellite images covering the Earth. Challenges are numerous: finding good features to distinguish objects, obtaining fine-resolution segmentations, while dealing with badly-registered groundtruth, keeping a scalable complexity, while avoiding boundary effects when tiling a big image into small ones, which are processed independently and merged back together. We propose to move to fully convolutional neural networks [45] to avoid artifacts from patch-based approaches. We show the benefits of training first on imprecise groundtruth, which is available in large amounts, and then refining on precise but scarce groundtruth [13]. To further refine the segmentation, as convolutional networks tend to produce blurry outputs, we use recurrent neural networks to learn the partial differential equation (PDE) which would sharpen the segmentations, i.e. an iterative process taking into account the edges in the original image to locate precisely their boundaries and to sharpen them [67]. Finally, to benefit simultaneously from information at various resolutions, we design a new, more suitable architecture [68].
  We also started to work on medical image classification, in the long-term goal of automatic diagnosis, in collaboration with the Necker Hospital and the Inria start-up Therapixel, and on image labelling and representation, with the database editor company Armadillo, through the Adamme project (cf Section 9.2.1).
  In collaboration with the University of Barcelona, we organize a series of challenges in video analysis of human behavior (ChaLearn Looking at People series). Looking at People (LAP) is an area of research that deals with the problem of automatically recognizing people in images, detecting and describing body parts, inferring their spatial configuration, performing action/gesture recognition from still images or image sequences, often including multi-modal data. Any scenario where the visual or multi-modal analysis of people takes a key role is of interest to us within the field of Looking at People. We have been leaders in organizing challenges in this area since 2013 [10], [12], [36], organizing events sponsored by DARPA, NSF, Microsoft, Google, Facebook, NVIDIA, and others. In 2016 we organized follow up competitions on gesture recognition [52] and face aging [37] to advance the state-of-the-art in areas we had previously explored. We also organized two rounds of a completely new recognition on personality trait evaluation from short video clips [47], [34]. The purpose of this study is to evaluate whether human first impression judgements are consistent and reproducible. Such research could lead to device coaching curricula to help job applicants present themselved better and hiring managers to overcome unsubstantiated negative biases. The winners of the challenge used Deep Learning methods. The third place winners teamed up with the organizers to put together a demonstration system, which was shown at the NIPS conference(https://nips.cc/Conferences/2016/Schedule?showEvent=6314). Work performed in collaboration with UC Berkeley on fingerprint verification using Deep Learning was also presented in this demonstration.
- **Natural Gradients for Deep Learning** Deep learning is now established as a state-of-the-art technology for performing different tasks such as image or sequence processing. Nevertheless, much of the computational burden is spent on tuning the hyper-parameters. On-going work, started during the TIMCO project, is proposing, in the framework of Riemannian gradient descents, invariant algorithms for training neural networks that effectively reduce the number of arbitrary choices, e.g., affine transformations of the activation functions or shuffling of the inputs. Moreover, the Riemannian gradient descent algorithms perform as well as the state-of-the-art optimizers for neural networks, and are even faster for training complex models. The proposed approach is based on Amari's theory of information geometry and consists in practical and well-grounded approximations for computing the Fisher metric. The scope of this framework, going beyond Deep Learning, encompasses any class of statistical models. This year's contribution is a new, simple framework (both theoretical and practical) that allowed us to release a simpler implementation of these techniques in Torch (one of the main deep learning libraries in use) and demonstrate good performance on real data. We have also started to explore criteria from information geometry criteria for automating the construction and selection of network architectures themselves, a major problem

given the current trend towards highly complex, hand-built model architectures (P. Wolinski's PhD).

- **Training dynamical systems online without backtracking** with application to recurrent neural networks. The standard way to train recurrent neural networks and other systems that exhibit a temporal dynamical behavior involves "backpropagation through time", which as the name indicates goes backward in time and is unrealistic. Last year we proposed an algorithm to learn the parameters of a dynamical system in an online, memoryless setting, thus scalable and requiring no backpropagation through time, in a way guaranteed to be unbiased. This year we started to provide full convergence proofs for this algorithm (the first of their kind). Moreover Corentin Tallec (PhD) proposed a considerably simpler version of the algorithm keeping the same key mathematical properties, which now allows for a simple "black-box" implementation on top of any existing recurrent network model.

ASPI Project-Team

6. New Results

6.1. Central limit theorem for adaptive multilevel splitting

Participants: Frédéric Cérou, Arnaud Guyader, Mathias Rousset.

This is a collaboration with Bernard Delyon (université de Rennes 1).

In this work, we consider the adaptive multilevel splitting algorithm as a Fleming–Viot particle system: the particles are indexed by levels instead of time, and the associated states are given by first entrance into level sets, in a similar fashion as in [38]. A rigorous proof of a central limit theorem has been obtained in [24] for Fleming–Viot particle systems. The application to AMS (adaptive multilevel splitting) algorithm is in preparation.

6.2. An efficient algorithm for video super-resolution based on a sequential model

Participant: Patrick Héas.

This is a collaboration with Angélique Drémeau (ENSTA Bretagne, Brest) and Cédric Herzet (EPI FLUMINANCE, Inria Rennes–Bretagne Atlantique)

In [16], we propose a novel procedure for video super–resolution, that is the recovery of a sequence of high–resolution images from its low-resolution counterpart. Our approach is based on a "sequential" model (i.e., each high-resolution frame is supposed to be a displaced version of the preceding one) and considers the use of sparsity-enforcing priors. Both the recovery of the high–resolution images and the motion fields relating them is tackled. This leads to a large–dimensional, non-convex and non-smooth problem. We propose an algorithmic framework to address the latter. Our approach relies on fast gradient evaluation methods and modern optimization techniques for non-differentiable/non-convex problems. Unlike some other previous works, we show that there exists a provably-convergent method with a complexity linear in the problem dimensions. We assess the proposed optimization method on several video benchmarks and emphasize its good performance with respect to the state of the art.

6.3. Low–rank approximation and dynamic mode decomposition

Participant: Patrick Héas.

This is a collaboration with Cédric Herzet (EPI FLUMINANCE, Inria Rennes–Bretagne Atlantique)

Dynamic mode decomposition (DMD) has emerged as a powerful tool for analyzing the dynamics of non-linear systems from experimental datasets. Recently, several attempts have extended DMD to the context of low-rank approximations. This low-rank extension takes the form of a non–convex optimization problem. To the best of our knowledge, only sub–optimal algorithms have been proposed in the literature to compute the solution of this problem. In [26], we prove that there exists a closed-form optimal solution to this problem and design an effective algorithm to compute it based on singular value decomposition (SVD). Based on this solution, we then propose efficient procedures for reduced-order modeling and for the identification of the low-rank DMD modes and amplitudes. Experiments illustrates the gain in performance of the proposed algorithm compared to state-of-the-art techniques.

6.4. Model reduction from partial observations

Participant: Patrick Héas.

This is a collaboration with Angélique Drémeau (ENSTA Bretagne, Brest) and Cédric Herzet (EPI FLUMINANCE, Inria Rennes–Bretagne Atlantique)

In [25], we deal with model order reduction of parametric partial differential equations (PPDE). We consider the specific setup where the solutions of the PPDE are only observed through a partial observation operator and address the task of finding a good approximation subspace of the solution manifold. We provide and study several tools to tackle this problem. We first identify the best worst–case performance achievable in this setup and propose simple procedures to approximate this optimal solution. We then provide, in a simplified setup, a theoretical analysis relating the achievable reduction performance to the choice of the observation operator and the prior knowledge available on the solution manifold.

In [22], we focus on reduced modeling of dynamical systems, in an analogous partial observation setup. Assuming prior knowledge available, we provide a unified reduction framework based on an a posteriori characterisation of the uncertainties on the solution manifold. Relying on sequential Monte Carlo (SMC) samples, we provide a closed-form approximation of solutions to the problem of choosing an optimal Galerkin projection or an optimal low–rank linear approximation. Numerical results obtained for a standard geophysical model show the gain brought by exploiting this posterior information for building a reduced model.

6.5. Combining analog method and ensemble data assimilation

Participants: Thi Tuyet Trang Chau, François Le Gland, Valérie Monbet.

This is a collaboration with Pierre Ailliot (université de Bretagne Occidentale, Brest), Ronan Fablet and Pierre Tandéo (Télé´com Bretagne, Brest), Anne Cuzol (université de Bretagne Sud, Vannes) and Bernard Chapron (IFREMER, Brest).

Nowadays, ocean and atmosphere sciences face a deluge of data from spatial observations, in situ monitoring as well as numerical simulations. The availability of these different data sources offer new opportunities, still largely underexploited, to improve the understanding, modeling and reconstruction of geophysical dynamics. The classical way to reconstruct the space–time variations of a geophysical system from observations relies on data assimilation methods using multiple runs of the known dynamical model. This classical framework may have severe limitations including its computational cost, the lack of adequacy of the model with observed data, modeling uncertainties. In [60], we explore an alternative approach and develop a fully data—driven framework, which combines machine learning and statistical sampling to simulate the dynamics of complex system. As a proof concept, we address the assimilation of the chaotic Lorenz–63 model and imputation of missing data in multisite wind and rain time series. We demonstrate that a nonparametric sampler from a catalog of historical datasets, namely local linear regression, combined with a classical stochastic data assimilation scheme, the ensemble Kalman filter and the particular filter, reach state–of–the–art performances, without online evaluations of the physical model. The use of local regression instead of analog sampler allows to improve the performance of the filters.

6.6. Classification trees, functional data, applications in biology

Participants: Valérie Monbet, Audrey Poterie.

This is a collaboration with Jean–François Dupuy (INSA Rennes) and Laurent Rouvière (université de Haute Bretagne, Rennes).

Classification and discriminant analysis methods have grown in depths during the past 20 years. Fisher linear discriminant analysis (LDA) is the basic but standard approach. As the structure and dimension of the data becomes more complex in a wide range of applications, such as functional data, there is a need for more flexible nonparametric classification and discriminant analysis tools, especially when the ratio of learning sample size to number of covariates is low and the covariates are highly correlated and the covariance matrix is highly degenerated or when the large number of covariates are generally weak in predicting the class labels. For some data such as spectrometry data, only some parts of the observed curves are discriminant leading to groups of variables.

We proposed a classification tree based on groups of variables. Like usual tree-based methods, the algorithm partitions the feature space into M regions, by recursively performing binary splits. The main difference is that each split is based on groups of variables and the boundary between both classes is the hyperplane which minimizes the Bayes risk in the set generated by the selected group of variables. We demonstrate on several toy examples and real spectrometry data that the performances of the proposed tree groups algorithm are at least as good as the one of the standard CART algorithm and group Lasso logistic regression.

CQFD Project-Team

7. New Results

7.1. Computable approximations for continuous-time Markov decision processes on Borel spaces based on empirical measures

The following result has been obtained by J. Anselmi (Inria CQFD), F. Dufour (Inria CQFD) and T. Prieto-Rumeau.

We propose an approach for approximating the value function and computing an ε-optimal policy of a continuous-time Markov decision processes with Borel state and action spaces, with possibly unbounded cost and transition rates, under the total expected discounted cost optimality criterion. Under the assumptions that the controlled process satisfies a Lyapunov type condition and the transition rate has a density function with respect to a reference measure, together with piecewise Lipschitz continuity of the elements of the control model, one can approximate the original controlled process by a sequence of models that are computationally solvable. Convergence of the approximations takes place at an exponential rate in probability.

7.2. Decentralized Proportional Load Balancing

The following result has been obtained by J. Anselmi (Inria CQFD) and N. Walton.

Load balancing is a powerful technique commonly used in communication and computer networks to improve system performance, robustness and fairness. In this paper, we consider a general model capturing the performance of communication and computer networks, and on top of it we propose a decentralized algorithm for balancing load among multiple network paths. The proposed algorithm is inspired by the modus operandi of the processor-sharing queue and on each network entry point operates as follows: every time a unit of load completes its service on a path, it increases by one unit the load of that path and decreases by one unit the load of a path selected at random with probability proportional to the amount of load on each of the available paths. We develop a dynamical system to argue that our load-balancer achieves a desirable network-wide utility optimization.

7.3. Constrained and Unconstrained Optimal Discounted Control of Piecewise Deterministic Markov Processes

The following result has been obtained by O. Costa, F. Dufour (Inria CQFD), and A. B. Piunovskiy.

The main goal of this paper is to study the infinite-horizon expected discounted continuous-time optimal control problem of piecewise deterministic Markov processes with the control acting continuously on the jump intensity λ and on the transition measure Q of the process but not on the deterministic flow ϕ. The contributions of the paper are for the unconstrained as well as the constrained cases. The set of admissible control strategies is assumed to be formed by policies, possibly randomized and depending on the history of the process, taking values in a set valued action space. For the unconstrained case we provide sufficient conditions based on the three local characteristics of the process ϕ, λ, Q and the semicontinuity properties of the set valued action space, to guarantee the existence and uniqueness of the integro-differential optimality equation (the so-called Bellman–Hamilton–Jacobi equation) as well as the existence of an optimal (and δ-optimal, as well) deterministic stationary control strategy for the problem. For the constrained case we show that the values of the constrained control problem and an associated infinite dimensional linear programming (LP) problem are the same, and moreover we provide sufficient conditions for the solvability of the LP problem as well as for the existence of an optimal feasible randomized stationary control strategy for the constrained problem.

7.4. Approximate Kalman-Bucy filter for continuous-time semi-Markov jump linear systems

The following result has been obtained by B. Saporta and E. F. Costa.

The aim of this paper is to propose a new numerical approximation of the Kalman-Bucy filter for semi-Markov jump linear systems. This approximation is based on the selection of typical trajectories of the driving semi-Markov chain of the process by using an optimal quantization technique. The main advantage of this approach is that it makes pre-computations possible. We derive a Lipschitz property for the solution of the Riccati equation and a general result on the convergence of perturbed solutions of semi-Markov switching Riccati equations when the perturbation comes from the driving semi-Markov chain. Based on these results, we prove the convergence of our approximation scheme in a general infinite countable state space framework and derive an error bound in terms of the quantization error and time discretization step. We employ the proposed filter in a magnetic levitation example with markovian failures and compare its performance with both the Kalman-Bucy filter and the Markovian linear minimum mean squares estimator.

7.5. Investigation of asymmetry in E. coli growth rate

The following result has been obtained by B. Saporta in collaboration with B. Delyon, N. Krell and Lydia Robert.

The data we analyze derives from the observation of numerous cells of the bacterium Escherichia coli (E. coli) growing and dividing. Single cells grow and divide to give birth to two daughter cells, that in turn grow and divide. Thus, a colony of cells from a single ancestor is structured as a binary genealogical tree. At each node the measured data is the growth rate of the bacterium. In this paper, we study two different data sets. One set corresponds to small complete trees, whereas the other one corresponds to long specific sub-trees. Our aim is to compare both sets. This paper is accessible to post graduate students and readers with advanced knowledge in statistics.

7.6. Impulsive Control for Continuous-Time Markov Decision Processes: A Linear Programming Approach

The following result has been obtained by F. Dufour (Inria CQFD) and A. B. Piunovskiy.

In this paper, we investigate an optimization problem for continuous-time Markov decision processes with both impulsive and continuous controls. We consider the so-called constrained problem where the objective of the controller is to minimize a total expected discounted optimality criterion associated with a cost rate function while keeping other performance criteria of the same form, but associated with different cost rate functions, below some given bounds. Our model allows multiple impulses at the same time moment. The main objective of this work is to study the associated linear program defined on a space of measures including the occupation measures of the controlled process and to provide sufficient conditions to ensure the existence of an optimal control.

7.7. Conditions for the Solvability of the Linear Programming Formulation for Constrained Discounted Markov Decision Processes

The following result has been obtained by F. Dufour (Inria CQFD) and T. Prieto-Rumeau.

We consider a discrete-time constrained discounted Markov decision process (MDP) with Borel state and action spaces, compact action sets, and lower semi-continuous cost functions. We introduce a set of hypotheses related to a positive weight function which allow us to consider cost functions that might not be bounded below by a constant, and which imply the solvability of the linear programming formulation of the constrained MDP. In particular, we establish the existence of a constrained optimal stationary policy. Our results are illustrated with an application to a fishery management problem.

7.8. Spatio-temporal averaging for a class of hybrid systems and application to conductance-based neuron models

The following result has been obtained by A. Genadot (Inria CQFD).

We obtain a limit theorem endowed with quantitative estimates for a general class of infinite dimensional hybrid processes with intrinsically two different time scales and including a population. As an application, we consider a large class of conductance-based neuron models describing the nerve impulse propagation along a neural cell at the scales of ion channels.

7.9. A comparison of fitness-case sampling methods for genetic programming

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with Y. Martinez, E. Naredo, L. Trujillo, U. Lopez.

The canonical approach towards fitness evaluation in Genetic Programming (GP) is to use a static training set to determine fitness, based on a cost function averaged over all fitness-cases. However, motivated by different goals, researchers have recently proposed several techniques that focus selective pressure on a subset of fitness-cases at each generation. These approaches can be described as fitness-case sampling techniques, where the training set is sampled, in some way, to determine fitness. This paper shows a comprehensive evaluation of some of the most recent sampling methods, using benchmark and real-world problems for symbolic regression. The algorithms considered here are Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and a new sampling technique is proposed called Keep-Worst Interleaved Sampling (KW-IS). The algorithms are extensively evaluated based on test performance, overfitting and bloat. Results suggest that sampling techniques can improve performance compared with standard GP. While on synthetic benchmarks the difference is slight or none at all, on real-world problems the differences are substantial. Some of the best results were achieved by Lexicase Selection and KeepWorse-Interleaved Sampling. Results also show that on real-world problems overfitting correlates strongly with bloating. Furthermore, the sampling techniques provide efficiency, since they reduce the number of fitness-case evaluations required over an entire run.

7.10. Prediction of Expected Performance for a Genetic Programming Classifier

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with Y. Martínez, L. Trujillo and E. Galván-López.

The estimation of problem difficulty is an open issue in genetic programming (GP). The goal of this work is to generate models that predict the expected performance of a GP-based classifier when it is applied to an unseen task. Classification problems are described using domain-specific features, some of which are proposed in this work, and these features are given as input to the predictive models. These models are referred to as predictors of expected performance. We extend this approach by using an ensemble of specialized predictors (SPEP), dividing classification problems into groups and choosing the corresponding SPEP. The proposed predictors are trained using 2D synthetic classification problems with balanced datasets. The models are then used to predict the performance of the GP classifier on unseen real-world datasets that are multidimensional and imbalanced. This work is the first to provide a performance prediction of a GP system on test data, while previous works focused on predicting training performance. Accurate predictive models are generated by posing a symbolic regression task and solving it with GP. These results are achieved by using highly descriptive features and including a dimensionality reduction stage that simplifies the learning and testing process. The proposed approach could be extended to other classification algorithms and used as the basis of an expert system for algorithm selection.

7.11. Evolving Genetic Programming Classifiers with Novelty Search

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with E. Naredo, L. Trujillo, S. Silvac andLuis Muñoza.

Novelty Search (NS) is a unique approach towards search and optimization, where an explicit objective function is replaced by a measure of solution novelty. However, NS has been mostly used in evolutionary robotics while its usefulness in classic machine learning problems has not been explored. This work presents a NS-based genetic programming (GP) algorithm for supervised classification. Results show that NS can solve real-world classification tasks, the algorithm is validated on real-world benchmarks for binary and multiclass problems. These results are made possible by using a domain-specific behavior descriptor. Moreover, two new versions of the NS algorithm are proposed, Probabilistic NS (PNS) and a variant of Minimal Criteria NS (MCNS). The former models the behavior of each solution as a random vector and eliminates all of the original NS parameters while reducing the computational overhead of the NS algorithm. The latter uses a standard objective function to constrain and bias the search towards high performance solutions. The paper also discusses the effects of NS on GP search dynamics and code growth. Results show that NS can be used as a realistic alternative for supervised classification, and specifically for binary problems the NS algorithm exhibits an implicit bloat control ability.

7.12. Regularity and Matching Pursuit Feature Extraction for the Detection of Epileptic Seizures

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with E. Z-Floresa, L. Trujillo, A. Soteloa and L. N. Coriaa.

The neurological disorder known as epilepsy is characterized by involuntary recurrent seizures that diminish a patient's quality of life. Automatic seizure detection can help improve a patient's interaction with her/his environment, and while many approaches have been proposed the problem is still not trivially solved.

In this work, we present a novel methodology for feature extraction on EEG signals that allows us to perform a highly accurate classification of epileptic states. Specifically, Hölderian regularity and the Matching Pursuit algorithm are used as the main feature extraction techniques, and are combined with basic statistical features to construct the final feature sets. These sets are then delivered to a Random Forests classification algorithm to differentiate between epileptic and non-epileptic readings.

Several versions of the basic problem are tested and statistically validated producing perfect accuracy in most problems and 97.6% accuracy on the most difficult case. Comparison with existing methods: A comparison with recent literature, using a well known database, reveals that our proposal achieves state-of-the-art performance. The experimental results show that epileptic states can be accurately detected by combining features extracted through regularity analysis, the Matching Pursuit algorithm and simple time-domain statistical analysis. Therefore, the proposed method should be considered as a promising approach for automatic EEG analysis.

7.13. Probabilistic safety analysis of the collision between a space debris and a satellite with an island particle algorithm

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with C. Verge, J. Morio and J.C Dolado Perez.

Collision between satellites and space debris seldom happens, but the loss of a satellite by collision may have catastrophic consequences both for the satellite mission and for the space environment. To support the decision to trigger off a collision avoidance manoeuver, an adapted tool is the determination of the collision probability between debris and satellite. This probability estimation can be performed with rare event simulation techniques when Monte Carlo techniques are not enough accurate. In this chapter, we focus on analyzing the influence of different simulation parameters (such as the drag coefficient) that are set for to simplify the simulation, on the collision probability estimation. A bad estimation of these simulation parameters can strongly modify rare event probability estimations. We design here a new island particle Markov chain Monte Carlo algorithm to determine the parameters that, in case of bad estimation, tend to increase the collision probability value. This algorithm also gives an estimate of the collision probability maximum taking into account the likelihood of the parameters. The principles of this statistical technique are described throughout this chapter.

7.14. Particle association measures and multiple target tracking

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with J. Houssineau.

In the last decade, the area of multiple target tracking has witnessed the introduction of important concepts and methods, aiming at establishing principled approaches for dealing with the estimation of multiple objects in an efficient way. One of the most successful classes of multi-object filters that have been derived out of these new grounds includes all the variants of the Probability Hypothesis Density (phd) filter. In spite of the attention that these methods have attracted, their theoretical performances are still not fully understood. In this chapter, we first focus on the different ways of establishing the equations of the phd filter, using a consistent set of notations. The objective is then to introduce the idea of observation path, upon which association measures are defined. We will see how these concepts highlight the structure of the first moment of the multi-object distributions in time, and how they allow for devising solutions to practical estimation problems.

7.15. Exponential mixing properties for time inhomogeneous diffusion processes with killing

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with D. Villemonais.

We consider an elliptic and time-inhomogeneous diffusion process with time-periodic coefficients evolving in a bounded domain of Rd with a smooth boundary. The process is killed when it hits the boundary of the domain (hard killing) or after an exponential time (soft killing) associated with some bounded rate function. The branching particle interpretation of the non absorbed diffusion again behaves as a set of interacting particles evolving in an absorbing medium. Between absorption times, the particles evolve independently one from each other according to the diffusion semigroup; when a particle is absorbed, another selected particle splits into two offsprings. This article is concerned with the stability properties of these non absorbed processes. Under some classical ellipticity properties on the diffusion process and some mild regularity properties of the hard obstacle boundaries, we prove an uniform exponential strong mixing property of the process conditioned to not be killed. We also provide uniform estimates w.r.t. the time horizon for the interacting particle interpretation of these non-absorbed processes, yielding what seems to be the first result of this type for this class of diffusion processes evolving in soft and hard obstacles, both in homogeneous and non-homogeneous time settings.

7.16. On particle Gibbs Markov chain Monte Carlo models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with R. Kohn and F. Patras.

This result analyses a new class of advanced particle Markov chain Monte Carlo algorithms recently introduced by Andrieu, Doucet, and Holenstein (2010). We present a natural interpretation of these methods in terms of well known unbiasedness properties of Feynman-Kac particle measures, and a new duality with Feynman-Kac models. This perspective sheds new light on the foundations and the mathematical analysis of this class of methods. A key consequence is their equivalence with the Gibbs sampling of a (many-body) Feynman-Kac target distribution. Our approach also presents a new stochastic differential calculus based on geometric combinatorial techniques to derive non-asymptotic Taylor type series for the semigroup of a class of particle Markov chain Monte Carlo models around their invariant measures with respect to the population size of the auxiliary particle sampler. These results provide sharp quantitative estimates of the convergence rate of the models with respect to the time horizon and the size of the systems. We illustrate the direct implication of these results with sharp estimates of the contraction coefficient and the Lyapunov exponent of the corresponding samplers, and explicit and non-asymptotic L p -mean error decompositions of the law of the random states around the limiting invariant measure. The abstract framework developed in the article also allows the design of natural extensions to island (also called SMC^2) type particle methodologies. We illustrate this general framework and results in the context of nonlinear filtering, hidden Markov chain problems with fixed unknown parameters, and Feynman-Kac path- integration models arising in computational physics and chemistry.

7.17. Sequential Monte Carlo with Highly Informative Observations

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with L. Murray.

We propose sequential Monte Carlo (SMC) methods for sampling the posterior distribution of state-space models under highly informative observation regimes, a situation in which standard SMC methods can perform poorly. A special case is simulating bridges between given initial and final values. The basic idea is to introduce a schedule of intermediate weighting and resampling times between observation times, which guide particles towards the final state. This can always be done for continuous-time models, and may be done for discrete-time models under sparse observation regimes; our main focus is on continuous-time diffusion processes. The methods are broadly applicable in that they support multivariate models with partial observation, do not require simulation of the backward transition (which is often unavailable), and, where possible, avoid pointwise evaluation of the forward transition. When simulating bridges, the last cannot be avoided entirely without concessions, and we suggest an epsilon-ball approach (reminiscent of Approximate Bayesian Computation) as a workaround. Compared to the bootstrap particle filter, the new methods deliver substantially reduced mean squared error in normalising constant estimates, even after accounting for execution time. The methods are demonstrated for state estimation with two toy examples, and for parameter estimation (within a particle marginal Metropolis–Hastings sampler) with three applied examples in econometrics, epidemiology and marine biogeochemistry.

7.18. A duality formula for Feynman-Kac path particle models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with R. Kohn and F. Patras.

This result presents a new duality formula between genetic type genealogical tree based particle models and Feynman–Kac measures on path spaces. Among others, this formula allows us to design reversible Gibbs–Glauber Markov chains for Feynman–Kac integration on path spaces. Our approach yields new Taylor series expansions of the particle Gibbs–Glauber semigroup around its equilibrium measure w.r.t. the size of the particle system, generalizing the recent work of Andrieu, Doucet, and Holenstein [1]. We analyze the rate of convergence to equilibrium in terms of the ratio of the length of the trajectories to the number of particles. The analysis relies on a tree-based functional and combinatorial representation of a class of Feynman–Kac particle models with a frozen ancestral line. We illustrate the impact of these results in the context of Quantum and Diffusion Monte Carlo methods.

7.19. Non-Asymptotic Analysis of Adaptive and Annealed Feynman-Kac Particle Models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with F. Giraud.

Sequential and quantum Monte Carlo methods, as well as genetic type search algorithms can be interpreted as a mean field and interacting particle approximations of Feynman-Kac models in distribution spaces. The performance of these population Monte Carlo algorithms is strongly related to the stability properties of nonlinear Feynman-Kac semigroups. In this paper, we analyze these models in terms of Dobrushin ergodic coefficients of the reference Markov transitions and the oscillations of the potential functions. Sufficient conditions for uniform concentration inequalities w.r.t. time are expressed explicitly in terms of these two quantities. We provide an original perturbation analysis that applies to annealed and adaptive Feynman-Kac models, yielding what seems to be the first results of this kind for these types of models. Special attention is devoted to the particular case of Boltzmann-Gibbs measures' sampling. In this context, we design an explicit way of tuning the number of Markov chain Monte Carlo iterations with temperature schedule. We also design an alternative interacting particle method based on an adaptive strategy to define the temperature increments. The theoretical analysis of the performance of this adaptive model is much more involved as both the potential functions and the reference Markov transitions now depend on the random evolution on the particle model. The nonasymptotic analysis of these complex adaptive models is an open research problem. We initiate this study with the concentration analysis of a simplified adaptive models based on reference Markov transitions that coincide with the limiting quantities, as the number of particles tends to infinity.

7.20. Uniform stability of a particle approximation of the optimal filter derivative

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with A. Doucet and S.S. Singh.

Particle methods, also known as Sequential Monte Carlo methods, are a principled set of algorithms used to approximate numerically the optimal filter in nonlinear non-Gaussian state-space models. However, when performing maximum likelihood parameter inference in state-space models, it is also necessary to approximate the derivative of the optimal filter with respect to the parameter of the model. References [G. Poyiadjis, A. Doucet, and S. S. Singh, Particle methods for optimal filter derivative: Application to parameter estimation, in Proceedings of IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP) 5, Philadelphia, 2005, pp. 925–928 and G. Poyiadjis, A. Doucet, and S. S. Singh, Biometrika, 98 (2011), pp. 65–80] present an original particle method to approximate this derivative, and it was shown in numerical examples to be numerically stable in the sense that it did not deteriorate over time. In this paper we theoretically substantiate this claim. $\mathbb{L}_p$ bounds and a central limit theorem for this particle approximation are presented. Under mixing conditions these $\mathbb{L}_p$ bounds and the asymptotic variance are uniformly bounded with respect to the time index.

7.21. Combining clustering of variables and feature selection using random forests: the CoV/VSURF procedure

The following result has been obtained by M. Chavent, and J. Saracco in collaboration with R. Genuer.

High-dimensional data classification is a challenging problem. A standard approach to tackle this problem is to perform variables selection, e.g. using stepwise procedures or LASSO approches. Another standard way is to perform dimension reduction, e.g. by Principal Component Analysis (PCA) or Partial Least Square (PLS) procedures. The approach proposed in this paper combines both dimension reduction and variables selection. First, a procedure of clustering of variables (CoV) is used to built groups of correlated variables in order to reduce the redundancy of information. This dimension reduction step relies on the R package ClustOfVar which can deal with both numerical and categorical variables. Secondly, the most relevant synthetic variables (which are numerical variables summarizing the groups obtained in the first step) are selected with a procedure of variable selection using random forests (VSURF), implemented in the R package VSURF. Numerical performances of the proposed methodology called CoV/VSURF are compared with direct applications of VSURF or random forests (RF) on the original p variables. Improvements obtained with the CoV/VSURF procedure are illustrated on two simulated mixed datasets (cases $n > p$ and $n << p$) and on a real proteomic dataset.

7.22. An innovative approach combining animal performances, nutritional value and sensory quality of meat

The following result has been obtained by M. Chavent and J. Saracco in collaboration with M.P. Ellies.

This work sets out a methodological approach to assess how to simultaneously control together animal performances, nutritional value, sensory quality of meat. Seventy-one young bulls were characterized by 97 variables. Variables of each element were arranged into either 5 homogeneous Intermediate Scores (IS) or 2 Global Indices (GI) via a clustering of variables and analysed together by Principal Component Analysis (PCA). These 3 pools of 5 IS (or 2 GI) were analysed together by PCA to established the links existing among the triptych. Classification on IS showed no opposition between animal performances and nutritional value of meat, as it seemed possible to identify animals with a high butcher value and intramuscular fat relatively rich in polyunsaturated fatty acids. Concerning GI, the classification indicated that animal performances were negatively correlated with sensory quality. This method appeared to be a useful contribution to the management of animal breeding for an optimal trade-off between the three elements of the triptych.

7.23. BIG-SIR: a Sliced Inverse Regression approach for massive data

The following result has been obtained by J. Saracco (Inria CQFD) in collaboration with B. Liquet.

In a massive data setting, we focus on a semiparametric regression model involving a real dependent variable Y and a p-dimensional covariable X. This model includes a dimension reduction of X via an index $X'\beta$. The Effective Dimension Reduction (EDR) direction β cannot be directly estimated by the Sliced Inverse Regression (SIR) method due to the large volume of the data. To deal with the main challenges of analysing massive datasets which are the storage and computational efficiency, we propose a new SIR estimator of the EDR direction by following the “divide and conquer” strategy. The data is divided into subsets. EDR directions are estimated in each subset which is a small dataset. The recombination step is based on the optimisation of a criterion which assesses the proximity between the EDR directions of each subset. Computations are run in parallel with no communication among them. The consistency of our estimator is established and its asymptotic distribution is given. Exten- sions to multiple indices models, q-dimensional response variable and/or SIR α-based methods are also discussed. A simulation study using our edrGraphicalTools R package shows that our approach enables us to reduce the computation time and conquer the memory constraint problem posed by massive datasets. A combination of foreach and bigmemory R packages are exploited to offer efficiency of execution in both speed and memory. Finally, results are visualised using the bin-summarise-smooth approach through the bigvis R package

MATHRISK Project-Team

7. New Results

7.1. Systemic risk

Participants: Agnès Bialobroda Sulem, Andreea Minca [Cornell University)], Rui Chen.

Our objective is to study the magnitude of default contagion in a large financial system, in which banks receive benefits from their connections, and to investigate how the institutions choose their connectivities by weighing the default risk and the benefits induced by connectivity. We study two versions of the model. In the first version (static) the benefits are received at the end of the contagion. In this case, each bank either receives fixed benefits per link if it survives, otherwise its payoff is zero. In the second version, which is a dynamic model, banks receive cash-flows from their connections, spread over time. Effectively, these cash flows increase the threshold of the bank over the time of contagion. We call this model contagion with intrinsic recovery features. In the first model, there is no calendar time. In the second model, the cash flows arrive at a certain rate in calendar time, while the losses come with each revealed link. We thus need to relate the intensity of revealing a link with calendar time. Both models have new features compared to past literature. The most important feature is that banks choose their connectivities optimally. The second model is dynamic and introduces growth over time. Computing the magnitude of contagion in this case is challenging, and we provide an iterative solution for this.

7.2. Backward stochastic (partial) differential equations with jumps, optimal stopping and stochastic control with nonlinear expectation

Participants: Agnès Bialobroda Sulem, Roxana Dumitrescu, Marie-Claire Quenez [(Univ Paris 7)], Bernt Øksendal, Arnaud Lionnet.

7.2.1. Nonlinear pricing in imperfect financial markets with default.

We pursue the development of the theory of stochastic control and optimal stopping with nonlinear expectation induced by a nonlinear BSDE with (default) jump, and the application to nonlinear pricing in financial markets with default. To that purpose we have studied nonlinear BSDE with default and proved several properties for these equations. We have also addressed the case with ambiguity on the model, in particular ambiguity on the default probability. In this context, we study robust superhedging strategies for the seller of a game optimal stopping problem by proving some duality results, and characterize the robust seller's price of a game option as the value function of a *mixed generalized* Dynkin game.

7.2.2. Stochastic control of mean-field SPDEs with jumps

We study stochastic maximum principles, both necessary and sufficient, for SPDE with jumps with a general mean-field operator.

7.2.3. Numerical methods for Forward-Backward SDEs

The majority of the results on the numerical methods for FBSDEs relies on the global Lipschitz assumption, which is not satisfied for a number of important cases such as the Fisher-KPP or the FitzHugh-Nagumo equations. In a previous work, A. Lionnet with Gonzalo Dos Reis and Lukasz Szpruch showed that for BSDEs with monotone drivers having polynomial growth in the primary variable y, only the (sufficiently) implicit schemes converge. But these require an additional computational effort compared to explicit schemes. They have thus developed a general framework that allows the analysis, in a systematic fashion, of the integrability properties, convergence and qualitative properties (e.g. comparison theorem) for whole families of modified explicit schemes. These modified schemes are characterized by the replacement of the driver by a driver that depends on the time-grid, and converge to the original driver as the size of the time-steps goes to 0. The framework yields the convergence of some modified explicit scheme with the same rate as implicit schemes and with the computational cost of the standard explicit scheme [55].

7.3. Optimal transport

Participants: Aurélien Alfonsi, Benjamin Jourdain.

With J. Corbetta (postdoc financed by the chair financial risks), A. Alfonsi and B. Jourdain are interested in the time derivative of the Wasserstein distance between the marginals of two Markov processes. The Kantorovich duality leads to a natural candidate for this derivative. Up to the sign, it is the sum of the integrals with respect to each of the two marginals of the corresponding generator applied to the corresponding Kantorovich potential. For pure jump processes with bounded intensity of jumps, J. Corbetta, A. Alfonsi and B. Jourdain proved that the evolution of the Wasserstein distance is actually given by this candidate. In dimension one, they show that this remains true for Piecewise Deterministic Markov Processes [45].

7.4. Option Pricing and Calibration

7.4.1. Calibration of regime-switching local volatility models

Participant: Benjamin Jourdain.

By Gyongy's theorem, a local and stochastic volatility model is calibrated to the market prices of all call options with positive maturities and strikes if its local volatility function is equal to the ratio of the Dupire local volatility function over the root conditional mean square of the stochastic volatility factor given the spot value. This leads to a SDE nonlinear in the sense of McKean. Particle methods based on a kernel approximation of the conditional expectation, as presented by Guyon and Henry-Labordère (2011), provide an efficient calibration procedure even if some calibration errors may appear when the range of the stochastic volatility factor is very large. But so far, no existence result is available for the SDE nonlinear in the sense of McKean. In the particular case where the local volatility function is equal to the inverse of the root conditional mean square of the stochastic volatility factor multiplied by the spot value given this value and the interest rate is zero, the solution to the SDE is a fake Brownian motion. When the stochastic volatility factor is a constant (over time) random variable taking finitely many values and the range of its square is not too large, B. Jourdain and A. Zhou prove existence to the associated Fokker-Planck equation. Thanks to Figalli (2008), they then deduce existence of a new class of fake Brownian motions. They extend these results to the special case of the LSV model called Regime Switching Local Volatility, where the stochastic volatility factor is a jump process taking finitely many values and with jump intensities depending on the spot level. Under the same condition on the range of its square, they prove existence to the associated Fokker-Planck PDE. They finally deduce existence of the calibrated model by extending the results in Figalli (2008).

7.4.2. American options

Participant: Damien Lamberton.

With Mihail Zervos, D. Lamberton has worked on American options involving the maximum of the underlying asset. With Giulia Terenzi, he has been working on American options in Heston's model. They obtained results about existence and uniqueness for the associated variational inequality, in suitable weighted Sobolev spaces (see Feehan and co-authors for recent results on elliptic problems).

7.5. Dependence modeling

7.5.1. Estimation of the parameters of a Wishart process

Participants: Aurélien Alfonsi, Ahmed Kebaier, Clément Rey.

We have studied the Maximum Likelihood Estimator for the Wishart processes and in particular its convergence in the ergodic and in some non ergodic cases. In the non ergodic cases, our analysis rely on refined results on the Laplace transform for Wishart processes. Our work also extends the recent paper by Ben Alaya and Kebaier on the maximum likelihood estimation for the CIR process.

7.6. Numerical Probability

7.6.1. Parametrix method for reflected SDEs

With A. Kohatsu-Higa and M. Hayashi, Aurelien Alfonsi is investigating how to apply the parametrix method recently proposed by V. Bally and A. Kohatsu-Higa for reflected SDEs. This method allows them to obtain an unbiased estimator for expectations of general functions of the process.

7.6.2. Regularity of probability laws using an interpolation method

Participants: Vlad Bally, Lucia Caramellino.

This work was motivated by previous papers of Nicolas Fournier, J. Printemps, E. Clément, A. Debussche and V. Bally on the regularity of the law of the solutions of some equations with coefficients with little regularity - for example diffusion processes with Hölder coefficients (but also many other examples including jump type equations, Bolzmann equation or Stochastic PDE's). Since we do not have sufficient regularity the usual approach by Malliavin calculus fails in this framework. Then one may use an alternative idea which roughly speaking is the following: We approximate the law of the random variable X (the solution of the equation at hand) by a sequence $X(n)$ of random variables which are smooth and consequently we are able to establish integration by parts formulas for $X(n)$ and we are able to obtain the absolutely continuity of the law of $X(n)$ and to establish estimates for the density of the law of $X(n)$ and for its derivatives. Notice that the derivatives of the densities of $X(n)$ generally blow up - so we can not derive directly results concerning the density of the law of X. But, if the speed of convergence of $X(n)$ to X is stronger than the blow up, then we may obtain results concerning the density of the law of X. It turns out that this approach fits in the framework of interpolation spaces and that the criterion of regularity for the law of X amounts to the characterization of an interpolation space between a space of distributions and a space of smooth functions. Although the theory of interpolation spaces is very well developed and one already know to characterize the interpolation spaces for Sobolev spaces of positive and negative indices, we have not found in the (huge) literature a result which covers the problem we are concerned with. So, although our result may be viewed as an interpolation result, it is a new one. As an application we discussed the regularity of the law of a Wiener functional under a Hörmander type non degeneracy condition. These papers will appear in Annals of Probability.

7.6.3. Regularity of the solution of jump type equations

Continuing the above work we study, in collabration with Lucia Caramellino, the regularity of the solution of jump type equations. This subject has been extensively treated in the literarure using different hypothesis and different variants of Malliavin calculus adapted to equations with jumps. The case of Poisson Point measures with absolutely continuous intensity measure is already well understood with the paper of Bichteler, Garereux and Jacod in the 80's. But the case of discrete intensity measures is more subtle. In this case J. Picard has succeded to obtain regularity results using a variant of Malliavin Calculus based on finite differences. We work also in this framework but we do not use directly some variant of Malliavin calculus but we use an interpolation argument . These are still working papers.

7.6.4. An invariance principle for stochastic series (U- Statistics)

In collaboration with L. Caramellino we work on invariance principles for stochastic series of polynomial type. In the case of polynomials of degree one we must have the classical Central Limit Theorem (for random variables which are not identically distributed). For polynomials of higher order we are in the framework of the so called U statistics which have been introduced by Hoffdings in the years 1948 and which play an important role in modern statistics. Our contribution in this topic concerns convergence in total variation distance for this type of objects. We use abstract Malliavin calculus and more generally, the methods mentioned in the above paragraph.

TOSCA Project-Team

6. New Results

6.1. Probabilistic numerical methods, stochastic modelling and applications

Participants: Mireille Bossy, Nicolas Champagnat, Madalina Deaconu, Coralie Fritsch, Pascal Helson, Benoît Henry, Kouadio Jean Claude Kouaho, Antoine Lejay, Radu Maftei, Sylvain Maire, Paolo Pigato, Alexandre Richard, Denis Talay, Etienne Tanré, Milica Tomasevic, Denis Villemonais.

6.1.1. Published works and preprints

- M. Bossy with H. Quinteros (UChile) studied the rate of convergence of a symmetrized version of the Milstein scheme applied to the solution of one dimensional CEV type processes. They prove a strong rate of convergence of order one, recovering the classical result of Milstein for SDEs with smooth diffusion coefficient. In contrast with other recent results, the proof does not relies on Lamperti transformation, and it can be applied to a wide class of drift functions. Some numerical experiments and comparison with various other schemes complement the theoretical analysis that also applies for the simple projected Milstein scheme with same convergence rate ([14] accepted for publication in Bernoulli Journal).
- M. Bossy, R. Maftei, J.-P. Minier and C. Profeta worked on numerically determining the rate of convergence of the weak error for the discretised Langevin system with specular reflection conditions. The article [29] presents a discretisation scheme and offers a conjecture for the rate of convergence of the bias produced. Numerically, these conjectures are confirmed for the specular reflection scheme but also for the absorption scheme, which models perfect agglomeration. The scheme numerically follows a linear decrease. The Richardson-Romberg extrapolation is also presented with a quadratic decrease.
- M. Bossy, A. Rousseau (LEMON Inria team), JĖspina, JṀorice and C. Paris (Inria Chile) studied the computation of the wind circulation around mills, using a Lagrangian stochastic approach. They present the SDM numerical method and numerical experiments in the case of non rotating and rotating actuator disc models in [13]. First, for validation purpose they compare some numerical experiments against wind tunnel measurements. Second, they perform numerical experiments at the atmospheric scale and present some features of the numerical method, in particular the computation of the probability distribution of the wind in the wake zone, as a byproduct of the fluid particle model and the associated PDF method.
- Together with M. Baar and A. Bovier (Univ. Bonn), N. Champagnat studied the adaptive dynamics of populations under the assumptions of large population, rare and small mutations [11]. In this work, the three limits are taken simultaneously, contrary to the classical approach, where the limits of large population and rare mutations are taken first, and next the limit of small mutations [57]. We therefore obtain the precise range of parameters under which these limits can be taken, and provide explicit biological conditions for which our approximation is valid.
- N. Champagnat and J. Claisse (Ecole Polytechnique) studied the ergodic and infinite horizon controls of discrete population dynamics with almost sure extinction in finite time. This can either correspond to control problems in favor of survival or of extinction, depending on the cost function. They have proved that these two problems are related to the QSD of the processes controled by Markov controls [36].
- N. Champagnat and C. Fritsch worked with F. Campillo (Inria Sophia-Antipolis, LEMON team) on the links between a branching process and an integro-differential equation of a growth-fragmentation-death model [15]. They proved that the two representations of the model lead to the same criteria of invasion of a population in a given environment. They also studied the variations of the principal eigenvalue (resp. the survival probability) of an integro-differential equation (resp. branching process) of growth-fragmentation models with respect to an environmental parameter in [35].

- N. Champagnat and D. Villemonais consider, for general absorbed Markov processes, the notion of quasi-stationary distributions (QSD), which is a stationary distribution conditionally on non-absorbtion, and the associated Q-process, degammad as the original Markov process conditioned to never be absorbed. They prove that, under the conditions of [17], in addition to the uniform exponential convergence of conditional distributions to a unique QSD and the uniform exponential ergodicity of the Q-process, one also has the uniform convergence of the law of the process contionned to survival up to time T, when $T \to +\infty$. This allows them to obtain conditional ergodic theorems [41].
- N. Champagnat, K. Coulibaly-Pasquier (Univ. Lorraine) and D. Villemonais obtained general criteria for existence, uniqueness and exponential convergence in total variation to QSD for multi-dimensional diffusions in a domain absorbed at its boundary [37]. These results improve and simplify the existing results and methods.
- Using a new method to compute the expectation of an integral with respect to a random measure, N. Champagnat and B. Henry obtained explicit formulas for the moments of the frequency spectrum in the general branching processes known as Splitting Trees, with neutral mutations and under the infinitely-many alleles model [16]. This allows them to obtain a law of large numbers for the frequency spectrum in the limit of large time.
- N. Champagnat and D. Villemonais obtained criteria for existence, uniqueness and exponential convergence in total variation to QSD for discrete population processes with unbounded absorption rate, using a non-linear Lyapunov criterion [38]. For logistic multidimensional birth and death processes absorbed when one coordinate gets extinct, they show that their criterion covers cases stronger intra-spectific competition than inter-specific competition.
- N. Champagnat and D. Villemonais extended their work [17] to general penalized processes, including time-inhomogeneous Markov processes with absorption and Markov processes in varying environments [40]. Their method allows to improve significantly the former results of [58], [59].
- M. Deaconu worked with L. Beznea and O. Lupaşcu (Bucharest, Romania) and analyzed the description of rupture phenomena like avalanches, by using fragmentation models. The main physical properties of the model are deeply involved in this study. They obtained new results on a stochastic equation of fragmentation and branching processes related to avalanches [12].
- M. Deaconu and S. Herrmann continued and completed the study of the simulation of hitting times of given boundaries for Bessel processes. These problems are of great interest in many application fields, such as finance and neurosciences. In a previous work, the authors introduced a new method for the simulation of hitting times for Bessel processes with integer dimension. The method was based mainly on explicit formula for the distribution of the hitting times and on the connexion between the Bessel process and the Euclidean norm of the Brownian motion. The method does not apply for a non-integer dimension. In this new work they consider the simulation of the hitting time of Bessel processes with non integer dimension and provide a new algorithm by using the additivity property of the laws of squared Bessel processes. Each simulation step is splitted in two parts: one is using the integer dimension case and the other one exhibits hitting time of a Bessel process starting from zero [20].
- M. Deaconu and S. Herrmann studied the Initial-Boundary Value Problem for the heat equation and solved it by using a new algorithm based on a random walk on heat balls [44]. Even if it represents a sophisticated and challenging generalization of the Walk on Spheres (WOS) algorithm introduced to solve the Dirichlet problem for Laplace's equation, its implementation is rather easy. The definition of the random walk is based on a new mean value formula for the heat equation. The convergence results and numerical examples allow to emphasize the efficiency and accuracy of the algorithm.
- M. Deaconu, B. Dumortier and E. Vincent (EPI MULTISPEECH are working with the Venathec SAS on the acoustic control of wind farms. They constructed a new approach to control wind farms based on real-time source separation. They expressed the problem as a non-linear knapsack problem and solve it using an efficient branch-and-bound algorithm that converges asymptotically to the global

optimum. The algorithm is initialised with a greedy heuristic that iteratively downgrades the turbines with the best acoustical to electricity loss ratio. The solution is then regammad using a depth-first search strategy and a bounding stage based on a continuous relaxation problem solved with an adapted gradient algorithm. The results are evaluated using data from 28 real wind farms [46].

- C. Fritsch and B. Cloez (INRA, Montpellier) proved central limit theorems for chemostat models in finite and infinite dimensions in [42]. From these theorems, they obtianed gaussian approximations of individual-based models and made a numerical analysis for the model in finite dimension in order to discuss the validity of these approximations in different contexts.
- Together with R. Azaïs (BIGS Inria team) and A. Genadot (Univ. Bordeaux), B. Henry studied an estimation problem for a forest of size-constrained Galton-Watson trees [31]. Using the asymptotic behavior of the Harris contour process, they constructed estimators for the inverse standard deviation of the birth distribution. In addition to the theoretical convergence results obtained in this work, they used the method to study the evolution of Wikipedia webpages in order, for instance, to detect vandalism.
- In [49], B. Henry showed a central limit theorem for the population counting process of a supercritical Splitting Tree in the limit of large time. Thanks to the results of [16], he also obtained a central limit theorem for the frequency spectrum of Splitting Trees with neutral mutations and under the infinitely-many alleles model.
- In collaboration with Laure Coutin, A. Lejay have studied the sensitivity of solution of rough differential equations with respect to their parameters using a Banach space version of the implicit function theorem. This result unifies and extends all the similar results on the subject [43].
- A. Lejay have studied the parametric estimation of the bias coefficient of skew random walk, as a toy model for the problem of estimation of the parameter of the Skew Brownian motion [50].
- P. Pigato has continued with V. Bally (Univ. Marne-la-Vallée) and L. Caramellino (Univ. Roma Tor Vergata) his PhD work on the regularity of diffusions under Hörmander-type conditions [32], [33].
- A. Richard and D. Talay ended their work on the sensitivity of the first hitting time of fractional SDEs, when $H > \frac{1}{2}$ [54]. This study is being completed by the rough case $H \in (\frac{1}{4}, \frac{1}{2}]$. In relation to fractional SDEs, another short work on accurate Gaussian-like upper bounds on density of one-dimensional fractional SDEs is almost finished.
- In [21], S. Herrmann and E. Tanré propose a new algorithm to simulate the first hitting times of a deterministic continuous function by a one-dimensional Brownian motion. They give explicit rate of convergence of the algorithm.
- E. Tanré and Pierre Guiraud (Univ. of Valparaiso) have studied the synchronization in a model of neural network with noise. Using a large deviation principle, they prove the stability of the synchronized state under stochastic perturbations. They also give a lower bound on the probability of synchronization for networks which are not initially synchronized. This bound shows the robustness of the emergence of synchronization in presence of small stochastic perturbations. [48]
- V. Reutenauer and E. Tanré have worked on extensions of the exact simulation algorithm introduced by Beskos et al. [56]. They propose an unbiased algorithm to approximate the two first derivatives with respect to the initial condition x of quantities with the form $\mathbb{E}\Psi(X_T^x)$, where X is a one-dimensional diffusion process and Ψ any test-function. They also propose an efficient modification of Beskos et al. algorithm. [53]
- During his internship supervised by E. Tanré, A. Papic worked on multi scales generator of Markov processes. He presents a method to approximate such processes with an application in neuroscience for noisy Hodgkin-Huxley model [52].
- D. Villemonais worked with P. Del Moral (Univ. Sydney) on the conditional ergodicity of time inhomogeneous diffusion processes [45]. They proved that, conditionally on non extinction, an elliptic time-inhomogeneous diffusion process forgets its initial distribution exponentially fast. An interacting particle scheme to numerically approximate the conditional distribution is also provided.

- D. Villemonais worked with his Research Project student William Oçafrain (École des Mines de Nancy) on an original mean-field particle system [51]. They proved that the mean-field particle system converges in full generality toward the distribution of a conditioned Markov process, with applications to the approximation of the quasi-stationary distribution of piecewise deterministic Markov processes.

6.1.2. Other works in progress

- M. Bossy and R. Maftei are working on determining the rate of convergence of the weak error of a discretised scheme for the Langevin system with specular boundary reflection on the position. The velocity process allows for a bounded and smooth drift. In order to determine the optimal rate of convergence, the regularity of the associated PDE is required and also regularity results for the derivative of flow of the process w.r.t. the initial conditions.
- N. Champagnat and B. Henry are studying limits of small mutations in Lokta-Volterra type PDEs of population dynamics using probabilistic representations and large deviations.
- N. Champagnat, C. Fritsch and S. Billiard (Univ. Lille) are working on food web modeling.
- M. Deaconu and S. Herrmann are working on numerical approaches for hitting times of general stochastic differential equations.
- M. Deaconu, O. Lupaşcu and L. Beznea (Bucharest, Romania) worked on the numerical scheme for the simulation of an avalanche by using the fragmentation model. This work will be submitted soon.
- M. Deaconu, B. Dumortier and E. Vincent (EPI MULTISPEECH) work on handling uncertainties in the model of acoustic control of wind farms they develop, in order to design a stochastic algorithm based on filtering methods. They will submit another article to IEEE transaction on sustainable energy.
- C. Fritsch is working with F. Campillo (Inria Sophia-Antipolis, LEMON team) and O. Ovaskainen (Univ. Helsinki) about a numerical approach to determine mutant invasion fitness and evolutionary singular strategies using branching processes and integro-differential models. They illustrate this method with a mass-structured individual-based chemostat model.
- C. Fritsch is working with A. Gégout-Petit (Univ. Lorraine and sc Bigs team), B. Marçais (INRA, Nancy) and M. Grosdidier (INRA, Nancy) on a statistical analysis of a *Chalara fraxinea* model.
- B. Cloez (INRA Montpellier) and B. Henry started a work on the asymptotic behavior of splitting trees in random environment. In addition, they begin the study of scaling limits of splitting trees in varying environment.
- Together with Ernesto Mordecki (Universidad de la República, Uruguay) and Soledad Torres (Universidad de Valparaíso), A. Lejay is working on the estimation of the parameter of the Skew Brownian motion.
- A. Lejay, and P. Pigato are working on the estimation of the parameters of diffusions with discontinuous coefficients, with application to financial data.
- Together with Laure Coutin and Antoine Brault (Université Toulouse 3), A. Lejay is studying application of the Trotter-Kato theorem in the context of rough differential equations, in order to solve some Stochastic Partial Differential Equations.
- A. Lejay and H. Mardones are working on a Monte Carlo simulation of the Navier-Stokes equations which is based on a novel probabilistic representation due to F. Delbaen *et al.* [60].
- In a research visit to Chile, P. Pigato has worked with R. Rebolledo and S. Torres on the estimation of parameters of diffusions from the occupation time and the local time of the process.
- Together with Laure Coutin and Antoine Brault (Université Toulouse 3), A. Lejay is studying application of the Trotter-Kato theorem in the context of rough differential equations, in order to solve some Stochastic Partial Differential Equations.

- C. Graham (École Polytechnique) and D. Talay are polishing thesecond volume of their series on Mathematical Foundation of Stochastic Simulation to be published by Springer.
- In collaboration with J. Bion-Nadal (CNRS and École Polytechnique) D. Talay ended the first paper on an innovating calibration method for stochastic models belonging to a family of solutions to martingale problems. The methodology involves the introduction of a new Wasserstein-type distance and stochastic control problems. The manuscript is being finished.
- Motivated by the study of systems of non-linear PDE's by stochastic methods, M. Tomasevic and D. Talay studied a system of differential equations interacting through a singular kernel, depending on all the past of the solutions. They have proved the existence of a solution in the space of Lipschitz functions in short time interval and performed numerical simulations. In the same time, they studied a non-linear stochastic differential equation whose drift is given as a convolution of a singular kernel with the unknown one dimensional time marginals both in time and space. Combining probabilistic and PDE techniques, they are currently finishing the proof of the existence and uniqueness of a weak solution up to an arbitrary finite time horizon. Properties of the corresponding particle system (well-posedness and propagation of chaos) are also studied.
- A. Richard and E. Tanré's work with Patricio Orio (CINV, Chile) on the modelling and measurement of long-range dependence in neuronal spike trains is almost completed. They exhibit evidence of memory effect in genuine neuronal data and compared their fractional integrate-and-fire model with the existing Markovian models. A. Richard and E. Tanré are still working on the convergence of the statistical estimator that measures this phenomenon.
- A. Richard, E. Tanré are working with S. Torres (Universidad de Valparaíso, Chile) on a one-dimensional fractional SDE reflected on the line. The existence and uniqueness of this process is known in the case $H > \frac{1}{2}$. In addition, they have proved the existence of a penalization scheme (suited to numerical approximation) to approach this object. When $H \in (\frac{1}{4}, \frac{1}{2})$, they have proved the existence in the elliptic case and are working on the question of uniqueness and on the relaxation of ellipticity.
- During his internship supervised by E. Tanré and Romain Veltz (MATHNEURO team), Pascal Helson studied numerically and theoretically a model of spiking neurons in interaction with plasticity. He showed that a simple model without plasticity could reproduce biological phenomena such as oscillations. In order to add plasticity, he enabled synaptic weights to evolve in a probabilistic way, in agreement with biological laws. He is now studying the convergence of this model and the existence of separable time scales, which is part of his thesis.
- D. Villemonais started a collaboration with Camille Coron (Univ. Paris Sud) and Sylvie Méléard (École Polytechnioque) on the question of simultaneous/non-simultaneous extinction of traits in a structured population
- D. Villemonais currently works on the computation of lower bounds for the Wasserstein curvature of interacting particle systems.
- D. Villemonais started a collaboration with Éliane Albuisson (CHRU of Nancy), Athanase Benetos (CHRU of Nancy), Simon Toupance (CHRU of Nancy), Daphné Germain (École des Mines de Nancy) and Anne Gégout-Petit (Inria BIGS team). The aim of this collaboration is to conduct a statistical study of the time evolution of telomere's length in human cells.

6.2. Financial Mathematics

Participants: Maxime Bonelli, Mireille Bossy, Nicolas Champagnat, Madalina Deaconu, Antoine Lejay, Sylvain Maire, Khaled Salhi, Denis Talay, Etienne Tanré.

6.2.1. Published works and preprints

- K. Salhi, M. Deaconu, A. Lejay and N. Champagnat worked with N. Navet (University of Luxembourg) [28]. They construct a regime switching model for the univariate Value-at-Risk estimation. Extreme value theory (EVT) and hidden Markov models (HMM) are combined to estimate a hybrid model that takes volatility clustering into account. In the first stage, HMM is used to classify data in crisis and steady periods, while in the second stage, EVT is applied to the previously classified data to rub out the delay between regime switching and their detection. This new model is applied to prices of numerous stocks exchanged on NYSE Euronext Paris over the period 2001-2011. The relative performance of the regime switching model is benchmarked against other well-known modeling techniques, such as stable, power laws and GARCH models.
- K. Salhi wrote a survey paper about option pricing and risk management under exponential Lévy models [55]. He detailed some notions that are not well explained in the literature and he proposed new trends in the risk management of derivatives.
- In [26], D. Talay, E. Tanré, Christophe Michel (CA-CIB) and Victor Reutenauer (fotonower) have studied a model in financial mathematics including bid-ask spread cost. They study the optimal strategy to hedge an interest rate swap that pays a fixed rate against a floating rate. They present a methodology using a stochastic gradient algorithm to optimize strategies.

6.2.2. Other works in progress

- M. Bossy and M. Bonelli (Koris International) are working on the optimal portfolio investment problem under the drawdown constraint that the wealth process never falls below a fixed fraction of its running maximum. They derive optimal allocation programs by solving numerically the Hamilton-Jacobi-Bellman equation that characterizes the finite horizon expected utility maximization problem, for investors with power utility as well as S-shape utility. Using numerical experiments they show that implementing the drawdown constraint can be gainful in optimal portfolios for the power utility, for some market configurations and investment horizons. However, their study reveals different results in a prospect theory context.
- When the underlying asset price is given by a exponential Lévy model, the market is almost incomplete. Under this hypothesis, K. Salhi works on derivatives hedging under a budget constraint on the initial capital. He considers, as criterion of optimization, the CVaR of the terminal hedging risk. First, he rewrites the problem an optimisation problem on the random fraction of the payoff that permits to respect the budget constraint. Then, he approximates the problem by relaxing the constraint and considering only a specific equivalent martingale measure. This approximate problem is solved using Neyman-Pearson's Lemma and, in the case of European options, a numerical valuation of the approximated minimal CVaR based on fast Fourier transform. The article will be submitted soon.