

**RESEARCH CENTER** 

FIELD Applied Mathematics, Computation and Simulation

# Activity Report 2017

# **Section New Results**

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## **ACUMES Project-Team**

## 6. New Results

### 6.1. Macroscopic traffic flow models on networks

**Participants:** Guillaume Costeseque, Nikodem Dymski, Paola Goatin, Nicolas Laurent-Brouty, Giulia Piacentini, Florent Berthelin [COFFEE, Inria], Antonella Ferrara [U Pavia, Italy], Simone Göttlich [U Mannheim, Germany], Oliver Kolb [U Mannheim, Germany].

In [38], we propose a new mathematical model accounting for the boundedness of traffic acceleration at a macroscopic scale. Our model is built on a first order macroscopic PDE model coupled with an ODE describing the trajectory of the leader of a platoon accelerating at a given constant rate. We use Wave Front Tracking techniques to construct approximate solutions to the Initial Value Problem. We present some numerical examples including the case of successive traffic signals on an arterial road and we compare the solution to our model with the solution given by the classical LWR equation in order to evaluate the impact of bounded acceleration.

The internship of Giulia Piacentini focused on traffic control via moving bottleneck of coordinated vehicles [35]. The possibility of properly controlling a moving bottleneck to improve the traffic flow was considered. The traffic is represented by means of a macroscopic model able to take into account the interactions with the bottleneck. This latter interacts with the surrounding flow modifying the traffic density and the flow speed profiles. An optimal control problem is stated by using the speed of the moving bottleneck as control variable. Specifically in this paper the MPC (Model Predictive Control) approach is used in order to get a fuel consumption reduction when the traffic is congested due to the presence of a fixed bottleneck on the highway. In addition we have demonstrated that no increase of the travel time is caused by the control application. The concept illustrated in this paper suggests a future innovative traffic control approach. Indeed the prospective of exploiting special vehicles with manipulable speed to control the traffic flow is particularly attractive given the expected increasing penetration rate of autonomous vehicles in traffic networks in future years.

In collaboration with S. Göttlich and O. Kolb, we studied macroscopic traffic flow models on a road network [36]. More precisely, we consider coupling conditions at junctions for the Aw-Rascle-Zhang second order model consisting of a hyperbolic system of two conservation laws. These coupling conditions conserve both the number of vehicles and the composition of traffic through the junction. The proposed Riemann solver is based on assignment coefficients, multi-objective optimization of fluxes and priority parameters. We prove that this Riemann solver is well posed in the case of special junctions, including 1-to-2 diverge and 2-to-1 merge.

In the setting of Florent Berthelin's secondement, we rigorously proved the convergence of the micro-macro limit for particle approximations of the Aw-Rascle-Zhang equations with a maximal density constraint [4]. The lack of BV bounds on the density variable is supplied by a compensated compactness argument.

### 6.2. Non-local conservation laws

Participants: Felisia Angela Chiarello, Paola Goatin, Elena Rossi.

F.A. Chiarello's PhD thesis focuses on non-local conservation laws. As a first result, we proved the wellposedness of entropy weak solutions for a class of scalar conservation laws with non-local flux arising in traffic modeling. We approximate the problem by a Lax-Friedrichs scheme and we provide  $L^{\infty}$  and BV estimates for the sequence of approximate solutions. Stability with respect to the initial data is obtained from the entropy condition through the doubling of variable technique. The limit model as the kernel support tends to infinity is also studied. See [33].

## 6.3. Crowd motion modeled by Fokker-Planck constrained Nash games

Participants: Alfio Borzí [Univ. Wurzburg], Abderrahmane Habbal, Souvik Roy [Univ. Wurzburg].

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 [48] a FPK-constrained control framework, where the drift was considered as control variable is developed and applied to crowd motion.

In [13] a new approach to modelling pedestrians' avoidance dynamics based on a Fokker–Planck (FP) Nash game framework is presented. In this framework, two interacting pedestrians are considered, whose motion variability is modelled through the corresponding probability density functions (PDFs) governed by FP equations. Based on these equations, a Nash differential game is formulated where the game strategies represent controls aiming at avoidance by minimizing appropriate collision cost functionals. The existence of Nash equilibria solutions is proved and characterized as a solution to an optimal control problem that is solved numerically. Results of numerical experiments are presented that successfully compare the computed Nash equilibria to the output of real experiments (conducted with humans) for four test cases.

# 6.4. Solving with games the coupled problem of conductivity or obstacle identification and data recovery

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

Based on previous successful attempts [104], [113] to tackle ill posed inverse problems a Nash games, we consider two developments :

The first one is related to joint obstacle shape/location and data recovery. We consider a game theory approach to deal with a geometric inverse problem related to the Stokes system. The problem consists in detecting an obstacle in a flow from incomplete measurements on the boundary of a domain. The approach that we propose deals simultaneously with the reconstruction of the missing data and the identification of one or more objects immersed in a viscous and incompressible fluid flow. The solution is interpreted in terms of Stackelberg-Nash equilibrium between both problems. We develop a new obstacle detection algorithm and we consider different numerical situations to illustrate the efficiency and robustness of the method.

The second one is dedicated to the electrocardiography inverse problem. 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 the data completion (heart electrical signal recovery) and conductivity identification at the same time.

## 6.5. The Kalai-Smorodinski solution for many-objective Bayesian optimization

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

Bayesian optimization methods are efficient to find solutions of multi-objective problems under very limited budgets of evaluation. An ongoing scope of research in multi-objective Bayesian optimization is to extend its applicability to a large number of objectives.

We have proposed in [127] 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.

Regarding the harsh many-objective optimization problems, the recovering of the set of optimal compromise solution generally requires lots of observations while being less interpretable, since this set tends to grow larger with the number of objectives. We thus propose to focus on a choice of a specific solution originating from game theory, the Kalai-Smorodinski solution, that possesses attractive properties [22] [19]. We further make it insensitive to a monotone transformation of the objectives by considering the objectives in the copula space. A tailored algorithm is proposed to search for the solution, which is tested on a synthetic problem.

## 6.6. Isogeometric analysis

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

We develop high-order isogeometric solvers, based on CAD representations for both geometry and solution space, for applications targeted by the team, in particular convection-dominated problems. Specifically, we investigate a Discontinuous Galerkin method for compressible Euler / Navier-Stokes 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 [34].

Recent extensions concern the capability to capture discontinuities in the solution, local refinement strategies by splitting algorithms [25] and high-order sensitivity analysis [24].

This topic is partially studied in A. Azaouzi's PhD work [21], [27], supervised by R. Duvigneau and M. Moakher.

### 6.7. 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 typical example the one-dimensional compressible Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach [20], [26], [32]. This study is achieved in collaboration with C. Chalons from University of Versailles, in the context of C. Florini's PhD work.

#### 6.8. Classification algorithms in Bayesian optimization

**Participants:** Régis Duvigneau, Matthieu Sacher [Ecole Navale], Frédéric Hauville [Ecole Navale], Olivier Le Maître [CNRS-LIMSI].

A Gaussian-Process based optimization algorithm is proposed to efficiently determine the global optimum for expensive simulations, when some evaluations may fail, due to unrealistic configurations, solver crash, degenerated mesh, etc. The approach is based on coupling the classical Bayesian optimization method with a classification algorithm, to iteratively identify the regions where the probability of failure is high.

The method is applied to the optimization of foils and sails in the context of racing yachts [14], [18], [23], [28], in particular for the America's Cup in collaboration with Groupama team. This work is part of M. Sacher's PhD work at Ecole Navale.

### 6.9. Multifidelity surrogate modeling based on Radial Basis Functions

**Participants:** Jean-Antoine Désidéri, Cédric Durantin [CEA Leti, University Côte d'Azur], Alain Glière [CEA Leti], Justin Rouxel [CEA Leti].

Multiple models of a physical phenomenon are sometimes available with different levels of approximation. The high fidelity model is more computationally 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 models. 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 does not bring better results than co-kriging but can be considered as an alternative for multifidelity metamodeling [9].

## 6.10. Descent algorithm for nonsmooth stochastic multiobjective optimization

**Participants:** Jean-Antoine Désidéri, Quentin Mercier [ONERA Châtillon, University Côte d'Azur], Fabrice Poirion [ONERA Châtillon].

An algorithm for solving the expectation formulation of stochastic nonsmooth multiobjective optimization problems is proposed. The proposed method is an extension of the classical stochastic gradient algorithm to multiobjective optimization using the properties of a common descent vector defined in the deterministic context. The mean square and the almost sure convergence of the algorithm are proven. The algorithm efficiency is illustrated and assessed on an academic example [12].

## 6.11. Hessian transfer for multilevel and adaptive shape optimization

**Participants:** Badr Abou el majd [Hassan II University Casablanca], Jean-Antoine Désidéri, Abderrahamane Habbal, Ouail Ouchetto [Hassan II University Casablanca].

We have developed a multilevel and adaption parametric strategies solved by optimization algorithms which require only the availability of objective function values but no derivative information. The key success of these hierarchical strategies refer to the quality of the downward and upward transfers of information. In this paper, we extend our approach when using a derivative-based optimization algorithms. The aim is to better re-initialize the Hessian and the gradient during the optimization process based on our construction of the downward and upward operators. The efficiency of this proposed approach is demonstrated by numerical experiments on an inverse shape model [1].

## **CAGIRE Project-Team**

## 7. New Results

## 7.1. Development of an accurate and stable finite volume scheme for simulating low Mach number flows with or without acoustic waves

Starting from the Roe scheme and various low Mach fixes for the barotropic Euler PDE's system and using a 2-scale asymptotic analysis of the (semi)-discrete system, a new Roe based scheme is derived whose set of dissipative terms is chosen in order to ensure both accuracy, stability and checkerboard free behaviour. A paper on this topic is being finalized.

## 7.2. Analysis of liquid sheet flowing under gravity

In the framework of an informal cooperation with Y. Le Guer and K. El Omari who are supervising the PhD thesis of A. Kacem, we have been involved in the experimental and the numerical study of liquid sheets falling under gravity [14]. The various flow regimes have been characterized in terms of the relevant dimensionless numbers (Weber, Reynolds, Ohnesorge) with a particular emphazis on the regimes leading to the appearance fo holes within the liquid sheet. A journal paper has been submitted mid-2017 and is presently under revision.

## 7.3. First order hyperbolic formulation of dissipative systems

In the framework of the leave of Vincent Perrier at National institute of Aerospace, a general framework for defining first order formulation of nonlinear dissipative systems equipped with an entropy has been developed. The numerical methods for discretizing this type of system are still in development.

### 7.4. Improvement of turbulent heat flux modelling for buoyant flows

Several modifications were introduced in the Elliptic Blending Differential Flux Model (EB-DFM) to account for the influence of wall blockage on the turbulent heat flux. These modifications are introduced in order to reproduce, in association with the most recent version of the EB-RSM, the full range of regimes, from forced to natural convection, without any case-specific modification. The interest of the new model is demonstrated using analytical arguments, a priori tests and computations in channel flows in the different convection regimes, as well as in a differentially heated cavity. This work is published in *Int. J. Heat Fluid Flow* [10].

# 7.5. Modelling of turbulent flows with strong variations of the physical properties

The effects of a strong transverse temperature gradient, very common in industrial applications, on a turbulent Poiseuille flow were studied numerically using RANS models, in order to determine the closure level necessary to reproduce the influence of variations of the physical properties, for a wide range of wall-temperature ratios. Eddy-viscosity models prove able to correctly reproduce the asymmetry of the flow and the tendency toward relaminarization close to the hot wall, which are mainly due to the strong variations of the molecular viscosity. Discrepancies in the predictions of the different closure levels only appear for the highest temperature ratios. A journal paper is under revision for publication in *Int. J. Heat Fluid Flow*.

## **CARDAMOM Project-Team**

## 7. New Results

#### 7.1. High order discretizations on unstructured meshes

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

A *p*-adaptive continuous residual distribution scheme has been proposed. Under certain conditions, primarily the expression of the total residual on a given element K into residuals on the sub-elements of K and the use of a suitable combination of quadrature formulas, it is possible to change locally the degree of the polynomial approximation of the solution. The discrete solution can then be considered non continuous across the interface of elements of different orders, while the numerical scheme still verifies the hypothesis of the discrete Lax–Wendroff theorem which ensures its convergence to a correct weak solution. The construction of our p-adaptive method has been done in the frame of a continuous residual distribution (RD) scheme. Different test cases for non-linear equations at different flow velocities demonstrate numerically the validity of the theoretical results.

As an evolution, a hp-adaptive RD scheme for the penalized Navier-Stokes equations has also been developed. The method combines hp-adaptation and penalization within a Residual Distribution scheme. The proposed method is an embedded boundary method that provides a simple and accurate treatment of the wall boundary conditions by the technique of penalization and anisotropic mesh adaptation. This method extends the IBM-LS-AUM method to higher order elements and is based on the construction of a p-adaptive RD scheme combined with an anisotropic mesh adaptation method. It has been applied to the resolution of the penalized Navier-Stokes equations. The robustness of the method is showed in practice with numerical experiments for different Mach regimes and Reynolds numbers in dimension two and three.

A novel formulation of residual distributions schemes as well as finite volume schemes on unstructured triangulations in curvilinear coordinates has been proposed within the PhD of L. Arpaia [31], generalising the work of [3]. The simulations reveal that the RD method proposed has very low dissipation when compared to the results existing in literature. This is very encouraging for applications in meteorology. A positivity preserving variant of the method has been used to compute large scale impact and inundation of the 2011 Tohoku tsunami [33], [32].

### 7.2. High order mesh generation and mesh adaptation

- Participants: Luca Arpaia, Cécile Dobrzynski, Marco Lorini, 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 proposed a new mixed model to compute the mesh deformations. This model is based on one hand on a Laplacian model and on the other hand on an Elasticity model. It takes advantages of the two approaches: a refined mesh where the solution varies a lot and a smooth gradation of the edges size elsewhere. We have applied this technic to 2d unsteady compressible simulations and we have preliminary results in three dimensions
- Additional work on *r*-adaptation has also involved a simple extension to spherical coordinates, allowing an efficient treatment of inundation caused by large scale tusnami waves [33], [32]

- A novel strategy to solve the finite volume discretization of the unsteady Euler equations within the ALE framework over tetrahedral adaptive grids have been proposed [11]. The volume changes due to local mesh adaptation are treated as continuous deformations of the finite volumes and they are taken into account by adding fictitious numerical fluxes to the governing equation. This peculiar interpretation enables to avoid any explicit interpolation of the solution between different grids and to compute grid velocities so that the GCL is automatically fulfilled also for connectivity changes. The solution on the new grid is obtained through standard ALE techniques, thus preserving the underlying scheme properties, such as conservativeness, stability and monotonicity. The adaptation procedure includes node insertion, node deletion, edge swapping and points relocation and it is exploited both to enhance grid quality after the boundary movement and to modify the grid spacing to increase solution accuracy. We have demonstrated the ability of the method on three-dimensional simulations of steady and unsteady flow fields.
- We extended our technique for generating high order curved meshes to immersed boundary problem. Based on a level-set function, we curved the mesh according to the 0-level-set. Preliminary results in 2d have been performed for compressible simulations
- Initial work on the use of fitting techniques to exactly compute moving shocks has been performed. The benefit of this approach in completely removing all numerical artefacts related to the capturing of the discontinuity, and in recovering the full order of accuracy have been shown for both straight and mildly curved discontinuities [42]

## 7.3. Uncertainty Quantification and robust design optimization

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

Concerning Uncertainty Quantification techniques, we have worked in three main directions. First, we developed novel techniques for building efficient and low-cost surrogate. In [43], two main points are introduced. Firstly, a technique which couples Universal Kriging with sparse Polynomial Dimensional Decomposition (PDD) to build a metamodel with improved accuracy. The polynomials selected by the adaptive PDD representation are used as a sparse basis to build an Universal Kriging surrogate model. The second is a strategy, derived from anisotropic mesh adaptation, to adaptively add a fixed number of new training points to an existing Design of Experiments. Moreover, we have explored in [44] how active subspaces are used to find a low-dimensional dependence structures in the input-to-output map of the forward numerical solver. Then, surrogate models on the active variables are used to accelerate the forward uncertainty propagation by Monte Carlo sampling and the Markov Chain Monte Carlo sampling of the posterior distribution for Bayesian inversion. Then, the forward and backward methodologies are applied to the simulation of a hypersonic flow around a cylinder, in conditions for which experimental data are available, revealing new insights towards the potential exploitation of heat flux data for freestream rebuilding.

The second action has been oriented towards the development of efficient techniques for computing lowprobability estimations. In [50], we have proposed a novel algorithm permitting to both building an accurate metamodel and to provide a statistically consistent error. In fact, it relies on a novel metamodel building strategy, which aims to refine the limit-state region in all the branches "equally", even in the case of multiple failure regions, with a robust stopping building criterion. Additionally, another importance sampling technique is proposed, permitting to drastically reduce the computational cost when estimating some reference values, or when a very weak failure-probability event should be computed directly from the metamodel.

Third, we have worked on the propagation of uncertainties through systems of solvers [25]. A System of Solvers (SoS) is a set of interdependent solvers where an output of an upstream solver can be the input of downstream solvers. In this work, we restrict ourselves to directed SoS with one-way dependences between solvers. Performing Uncertainty Quantification (UQ) analysis in SoS is challenging because it typically encapsulates a large number of uncertain input parameters and classical UQ methods, such as spectral expansions and Gaussian process models, are affected by the curse of dimensionality. In this work, we develop

an original mathematical framework, based on Gaussian Process (GP) models to construct a global surrogate model of the uncertain SoS, that can be used to solve forward and backward UQ problems. The key idea of the proposed approach is to determine a local GP model for each solver constituting the SoS. These local GP models are built adaptively to satisfy criteria based on the global output error estimation. The error estimate can be decomposed into contributions from the individual GP models, enabling one to select the GP models to refine to efficiently reduce the global error. The framework is first tested on several analytical problems and subsequently applied to space object reentry simulations.

Concerning optimization under uncertainties, we have worked on the formulation of novel framework to perform multi-objective optimization [24], when considering an error on the objective functions. In many engineering optimization problems, the objective functions are affected by an error arising from the model employed for the computation of the functions. For example, in the case of uncertainty-based optimization the objective functions are statistics of a performance of interest which is uncertain due to the variability of the system input variables. These estimated objectives are affected by an error, which can be modeled with a confidence interval. The framework proposed here is general and aims at dealing with any error affecting a given objective function. The strategy is based on the extension of the Bounding-Box concept to the Pareto optima, where the error can be regarded with the abstraction of an interval (in one-dimensional problems) or a Bounding-Box (in multi-dimensional problems) around the estimated value. This allows the computation of an approximated Pareto front, whose accuracy is strongly dependent on the acceptable computational cost. This approach is then supplemented by the construction of an evolutive surrogate model on the objective functions, iteratively refined during the optimization process. This allows ultimately to further reduce the computation cost of the Pareto front with approximations of the objective functions at a negligible cost. Regarding optimization, we have also worked on the formulation of a novel optimization under uncertainty framework for the definition of optimal shapes for morphing airfoils, applied here to advancing/retreating 2D airfoils. In particular, the morphing strategy is conceived with the intent of changing the shape at a given frequency to enhance aerodynamic performance. The optimization of morphing airfoils pre- sented here only takes into account the aerodynamic performance. The paper [5] is then focused on an aerodynamic optimization to set the optimal shape with respect to performance, where technological aspects are inserted through geometrical constraints.

## 7.4. Modelling of free surface flows

- Participants: Luca Arpaia, Mathieu Colin, Andrea Filippini, Maria Kazolea, Luc Mieussens, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

This year we continue our work on fully non-linear weakly dispersive wave models in two dimensional horizontal coordinates. The proposed framework in [92], to approximate the so-called 2D Green-Naghdi equations has been presented in ISOPE (citation) conference an new paper is under preparation.

We also continue our study on wave breaking techniques on BT models [48]. We studied weakly and fully nonlinear models representative of classical and well known models/codes such as BOUSS-2D [85], [86], Funwave [144], [129], Coulwave [109], [131], BOSZ [128], MIKE21 [83], TUCWave [100], [101], and others. We have in particular focused on the enhanced equations of Nwogu [117], and on a frequency enhanced version of the Green-Naghdi system in the form proposed in [69], [93]. We have compared the now popular hybrid closure initially proposed in [136], with an eddy viscosity closure based on an adaptation of the turbulent kinetic energy closure model of [118], modified to be consistent with the detection mechanisms proposed of [101], [93], and also used here. The study performed has involved: a systematic analysis of the behaviour of the two closures for different mesh sizes; the use of dissipation monitors, consistent with the available theory of entropy dissipation for conservation laws [132], [133], to study the dynamics of breaking for several cases; thorough evidence of the equivalent capabilities of the two approaches to provide satisfactory results. Our results indicate that indeed, at least with the (rather standard) implementation proposed here, both closure approaches allow to describe correctly wave transformation and breaking at large scales. We have shown that when using the TKE eddy viscosity closure the numerical dissipation plays a negligible role, which motivates

to look for non-dissipative/energy conserving numerical methods in the future. Also, the results clearly show the reduced sensitivity to the mesh of this approach compared to the hybrid one. The analysis of the wave breaking of solitary waves on a slope also has allowed to quantitatively study the interplay of the dissipation introduced by friction, eddy viscosity, and numerical dissipation. A research paper is under review.

Further more we continue our work for weakly non linear weakly dispersive models, 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 review.

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 [6], [140]. We also our code SLOWS, to study the conditions for tidal bore formation in convergent alluvial estuaries [70]. 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.

## 7.5. Wave energy conversion hydrodynamics

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

We have proposed an efficient nonlinear modelling tool for the analysis of wave body interaction based on Boussinesq-type equations. The approach develop here is based on a PDE formulation which model the flow under the body with a depth averaged system featuring an unknown pressure for which a Poisson type problem must solved by appropriately embedding the constraint on the position of the body. The PDE system is discretised by means of a high-order continuous spectral/hp element method in which the coupling between the free surface and floater domains is handled by means of numerical fluxes inspired by techniques used in the discontinuous Galerkin approach. The model is now fully validated both in the hydrostatic case and in the non-hydrostatic one [36], [37]. Several extensions are under way within the MIDWEST project.

## 7.6. Kinetic modelling of rarefied gases and space reentry

- Participants: Giorgio Martalò, Luc Mieussens, Julien Mathiaud
- Corresponding member: Luc Mieussens

After the end of the post-doc of Giorgio Martalò, a paper has been published [2], in which as presented the derivation of modified boundary conditions for the compressible Navier-Stokes equations to take into account rarefied flow effects. Another paper, related to some numerical aspects, should be submitted soon. Moreover, a paper written by J. Mathiaud and L. Mieussens [7]. This is an extension of their previous work on the modelling of collisions in gases by Fokker-Planck model to polyatomic gases.

Finally, Baranger et. al [53] have presented a way to obtain correct numerical boundary conditions for the approximation of the Boltzmann equation to take into account collisions of gas molecules with solid boundaries. Standard second order finite volume schemes degenerate to first order close to solid walls, but it has been shown in [53] that a suitable use of extrapolation and slope limiters can give second order accuracy. This greatly improves the computation of the heat flux on solid boundaries for atmospheric re-entry flow simulation, for instance.

Finally, the project of numerical and physical modelling of the liquid ablation (for atmospheric re-entry flows) has been concluded by the defense of Simon Peluchon in November 2017. So far, one paper has been published on this subject [8], but at least another one should be submitted soon. Note that Simon Peluchon will be hired in the CEA as a researcher-engineer in January 2018. This subject might induce new collaborations between the CEA and Cardamom, in particular for the use of unstructured grids.

We have developed some activities concerning the application of UQ analysis to aerospace problems. First, we have illustrated in [44] how to perform a Bayesian calibration of the free stream parameters of a hypersonic high-enthalpy flow around a cylinder, exploiting active subspaces for the reduction of the dimensionality of the input space. The configuration taken into account was the HEG I configuration, known in literature as a validation test-case for hypersonic CFD. The goal of the Bayesian inversion was to show the feasibility in using measurements of pressure and heat flux at the stagnation point for rebuilding freestream velocity and density.

Then, we have realized several studies concerning ablation and the characterization of ablative materials. In particular, in [16] and [15], we have illustrated a proof-of-concept of the coupling between a thermochemical ablation model and modern uncertainty quantification techniques with the aim of rebuilding the ablative material tests performed in the inductively coupled Plasmatron facility at the von Karman Institute. Finally, in [14], we have shown how an approach that uses uncertainty quantification methodology can be used in order to rigorously compute error bars on numerically rebuilt values of enthalpy and catalycity from the Plasmatron facility.

## 7.7. Modelling of icing/de-icing

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

The final public workshop of the European STORM project took place at the end of March 2017. The novel high-fidelity approach, based on penalization, proposed by Cardamom to model ice block trajectories has been compared to a low-fidelity approach from Airbus, to two chimera grids approaches from DLR and ONERA and to an experimental database elaborated during the project. The preliminary results are encouraging and commit to further developments of the method.

## **DEFI Project-Team**

## 6. New Results

#### 6.1. Methods for inverse problems

#### 6.1.1. The Generalized Linear Sampling Method for limited aperture measurements

#### L. Audibert and H. Haddar

We extend the so-called Generalized Linear Sampling Method (GLSM) to the case of limited aperture data at a fixed frequency. In this case the factorization of the sampling operator does not obey the symmetry required in the justification of the GLSM introduced in Audibert-Haddar [Inverse Problems, 2014]. We propose a new formulation by adding an extra penalty term that asymptotically correct the non symmetry of the GLSM original penalty term. The analysis of the new formulation is first presented in an abstract framework. We then show how to apply our setting to the scalar problem with far field measurements or near field measurements on a limited aperture. We finally validate the method through some numerical tests in two dimensions and for far field measurements.

## 6.1.2. A synoptic approach to the seismic sensing of heterogeneous fractures: from geometric reconstruction to interfacial characterization

#### B. Guzina, H. Haddar and F. Pourahmadian

A non-iterative waveform sensing approach is proposed toward (i) geometric reconstruction of penetrable fractures, and (ii) quantitative identification of their heterogeneous contact condition by seismic i.e. elastic waves. To this end, the fracture support  $\Gamma$  (which may be non-planar and unconnected) is first recovered without prior knowledge of the interfacial condition by way of the recently established approaches to non-iterative waveform tomography of heterogeneous fractures, e.g. the methods of generalized linear sampling and topological sensitivity. Given suitable approximation  $\Gamma$  of the fracture geometry, the jump in the displacement field across  $\Gamma$  i.e. the fracture opening displacement (FOD) profile is computed from remote sensory data via a regularized inversion of the boundary integral representation mapping the FOD to remote observations of the scattered field. Thus obtained FOD is then used as input for solving the traction boundary integral equation on  $\Gamma$  for the unknown (linearized) contact parameters. In this study, linear and possibly dissipative interactions between the two faces of a fracture are parameterized in terms of a symmetric, complex-valued matrix K collecting the normal, shear, and mixed-mode coefficients of specific stiffness. To facilitate the high-fidelity inversion for K, a 3-step regularization algorithm is devised to minimize the errors stemming from the inexact geometric reconstruction and FOD recovery. The performance of the inverse solution is illustrated by a set of numerical experiments where a cylindrical fracture, endowed with two example patterns of specific stiffness coefficients, is illuminated by plane waves and reconstructed in terms of its geometry and heterogeneous (dissipative) contact condition.

## 6.1.3. Sampling methods for reconstructing the geometry of a local perturbation in unknown periodic layers

#### H. Haddar and T.P Nguyen

The aim of this work is the design and analysis of sampling methods to reconstruct the shape of a local perturbation in a periodic layer from measurements of scattered waves at a fixed frequency. We first introduce the model problem that corresponds with the semi-discretized version of the continous model with respect to the Floquet-Bloch variable. We then present the inverse problem setting where (propagative and evanescent) plane waves are used to illuminate the structure and measurements of the scattered wave at a parallel plane to the periodicity directions are performed. We introduce the near field operator and analyze two possible factorizations of this operator. We then establish sampling methods to identify the defect and the periodic

background geometry from this operator measurement. We also show how one can recover the geometry of the background independently from the defect. We then introduce and analyze the single Floquet-Bloch mode measurement operators and show how one can exploit them to built an indicator function of the defect independently from the background geometry. Numerical validating results are provided for simple and complex backgrounds.

#### 6.1.4. Nanoparticles volume determination from SAXS measurements

#### M. Bakry and H. Haddar

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. The developement of this research topic is ongoing under the framework of Saxsize.

### 6.1.5. 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.

## **6.2.** Invisiblity and transmission eigenvalues

#### 6.2.1. Trapped modes and reflectionless modes as eigenfunctions of the same spectral problem

#### A.-S. Bonnet-Ben Dhia, L. Chesnel and V. Pagneux

We consider the reflection-transmission problem in a waveguide with obstacle. At certain frequencies, for some incident waves, intensity is perfectly transmitted and the reflected field decays exponentially at infinity. We show that such reflectionless modes can be characterized as eigenfunctions of an original non-selfadjoint spectral problem. In order to select ingoing waves on one side of the obstacle and outgoing waves on the other side, we use complex scalings (or Perfectly Matched Layers) with imaginary parts of different signs. We prove that the real eigenvalues of the obtained spectrum correspond either to trapped modes (or bound states in the continuum) or to reflectionless modes. Interestingly, complex eigenvalues also contain useful information on weak reflection cases. When the geometry has certain symmetries, the new spectral problem enters the class of PT-symmetric problems.

## 6.2.2. Transmission eigenvalues with artificial background for explicit material index identification

#### L. Audibert, L. Chesnel and H. Haddar

We are interested in the problem of retrieving information on the refractive index n of a penetrable inclusion embedded in a reference medium from farfield data associated with incident plane waves. Our approach relies on the use of transmission eigenvalues (TEs) that carry information on n and that can be determined from the knowledge of the farfield operator F. We explain how to modify F into a farfield operator  $F^a = F - \tilde{F}$ , where  $\tilde{F}$  is computed numerically, corresponding to well chosen artificial background and for which the associated TEs provide more accessible information on n.

#### 6.2.3. Simple examples of perfectly invisible and trapped modes in waveguides

#### L. Chesnel and V. Pagneux

We consider the propagation of waves in a waveguide with Neumann boundary conditions. We work at low wavenumber focusing our attention on the monomode regime. We assume that the waveguide is symmetric with respect to an axis orthogonal to the longitudinal direction and is endowed with a branch of height L whose width coincides with the wavelength of the propagating modes. In this setting, tuning the parameter L, we prove the existence of simple geometries where the transmission coefficient is equal to one (perfect invisibility). We also show that these geometries, for possibly different values of L, support so called trapped modes (non zero solutions of finite energy of the homogeneous problem) associated with eigenvalues embedded in the continuous spectrum.

#### 6.2.4. Invisibility and perfect reflectivity in waveguides with finite length branches

#### L. Chesnel, S.A. Nazarov and V. Pagneux

We consider a time-harmonic wave problem, appearing for example in water-waves theory, in acoustics or in electromagnetism, in a setting such that the analysis reduces to the study of a 2D waveguide problem with a Neumann boundary condition. The geometry is symmetric with respect to an axis orthogonal to the direction of propagation of waves. Moreover, the waveguide contains one branch of finite length. We analyse the behaviour of the complex scattering coefficients  $\mathcal{R}$ ,  $\mathcal{T}$  as the length of the branch increases and we exhibit situations where non reflectivity ( $\mathcal{R} = 0$ ,  $|\mathcal{T}| = 1$ ), perfect reflectivity ( $|\mathcal{R}| = 1$ ,  $\mathcal{T} = 0$ ) or perfect invisibility ( $\mathcal{R} = 0$ ,  $\mathcal{T} = 1$ ) hold. Numerical experiments illustrate the different results.

#### 6.2.5. 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  $k_{\overrightarrow{\lambda}}$  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),  $k_{\overrightarrow{\lambda}}$  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.

## 6.2.6. New sets of eigenvalues in inverse scattering for inhomogeneous media and their determination from scattering data

F. Cakoni, H. Haddar and L. Audibert

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We developed a general mathematical framework to determine interior eigenvalues from a knowledge of the modified far field operator associated with an unknown (anisotropic) inhomogeneity. The modified far field operator is obtained by subtracting from the measured far field operator the computed far field operator corresponding to a well-posed scattering problem depending on one (possibly complex) parameter. Injectivity of this modified far field operator is related to an appropriate eigenvalue problem whose eigenvalues can be determined from the scattering data, and thus can be used to obtain information about material properties of the unknown inhomogeneity. We discuss here two examples of such modification leading to a Steklov eigenvalue problem, and a new type of the transmission eigenvalue problem. We present some numerical examples demonstrating the viability of our method for determining the interior eigenvalues form far field data.

### 6.2.7. The Asymptotic of Transmission Eigenvalues for a Domain with a Thin Coating

#### H. Boujlida, H Haddar and M. Khenissi

We consider the transmission eigenvalue problem for a medium surrounded by a thin layer of inhomogeneous material with different refractive index. We derive explicit asymptotic expansion for the transmission eigenvalues with respect to the thickness of the thin layer. We prove error estimate for the asymptotic expansion up to order 1 for simple eigenvalues. This expansion can be used to obtain explicit expressions for constant index of refraction.

## 6.3. Shape and topology optimization

## 6.3.1. Structural optimization under overhang constraints imposed by additive manufacturing technologies

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

This work addresses one of the major constraints imposed by additive manufacturing processes on shape optimization problems - that of overhangs, i.e. large regions hanging over void without sufficient support from the lower structure. After revisiting the 'classical' geometric criteria used in the literature, based on the angle between the structural boundary and the build direction, we propose a new mechanical constraint functional, which mimics the layer by layer construction process featured by additive manufacturing technologies, and thereby appeals to the physical origin of the difficulties caused by overhangs. This constraint, as well as some variants, are precisely defined; their shape derivatives are computed in the sense of Hadamard's method, and numerical strategies are extensively discussed, in two and three space dimensions, to efficiently deal with the appearance of overhang features in the course of shape optimization processes.

## 6.3.2. Shape optimisation with the level set method for contact problems in linearised elasticity

#### G. Allaire, F. Jouve and A. Maury

This work is devoted to shape optimisation of contact problems in linearised elasticity, thanks to the level set method. We circumvent the shape non-differentiability, due to the contact boundary conditions, by using penalised and regularised versions of the mechanical problem. This approach is applied to five different contact models: the frictionless model, the Tresca model, the Coulomb model, the normal compliance model and the Norton-Hoff model. We consider two types of optimisation problems in our applications: first, we minimise volume under a compliance constraint, second, we optimise the normal force, with a volume constraint, which is useful to design compliant mechanisms. To illustrate the validity of the method, 2D and 3D examples are performed, the 3D examples being computed with an industrial software.

#### 6.3.3. Elasto-plastic shape optimization using the level set method

G. Allaire, F. Jouve and A. Maury

This work is concerned with shape optimization of structures made of a material obeying Hencky's laws of plasticity, with the stress bound expressed by the von Mises effective stress. The ill-posedness of the model is circumvented by using two regularized versions of the mechanical problem. The first one is the classical Perzyna formulation which is regularized, the second one is a new regularized formulation proposed for the von Mises criterion. Shape gradients are calculated thanks to the adjoint method. The optimal shape is numerically computed by using the level set method. To illustrate the validity of the method, 2D examples are performed.

## 6.4. Numerical methods for wave problems

#### 6.4.1. 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.

## 6.4.2. Linearized Navier-Stokes equations for Aeroacoustics using Stabilized Finite Elements : Boundary Conditions and Industrial Application to Aft-Fan Noise Propagation.

A. Bissuel, G. Allaire, L. Daumas, S., Barré and F. Rey

A numerical method for solving the linearized Navier-Stokes equations is presented for aeroacoustic sound propagation problem. The Navier-Stokes equations are linearized in the frequency domain. The fan noise of jet engine is emitted nearly selectively on some frequencies, which depend on the rotation velocity of the fan. A frequency domain approach is highly suitable for this kind of problems, instead of a costly time-dependent simulation which can handle a large range of frequencies depending on the time step and the mesh. The calculations presented here were all made using Aether, a Navier- Stokes code which uses finite elements stabilized with SUPG (Streamline Upwind Galerkin). Automatic code differentiation was used to linearize this code. Entropy variables bring interesting mathematical properties to the numerical scheme, but also prevent the easy implementation of boundary conditions. For instance, the pressure is a non-linear combination of the entropy variables. Imposing a pressure variation needs a linearization of this relation which is detailed herein. The performance of different types of boundary conditions used to impose the acoustic pressure variation inside the engine is studied in detail. Finally, a very surprising effect of the SUPG scheme was to transform a homogeneous Dirichlet boundary condition on all variables to a transparent one which is able to let only outgoing waves pass through with no incoming wave. A one-dimensional toy model is given to explain how SUPG brings about this transformation.

We finally treated an industrial test case. The geometry of a model turbine from the Clean Sky European project was used for sound propagation of the fan exhaust noise of a jet engine. Computations on several modes with increasing complexities were done and the results compared to a boundary element method which served as a reference when no mean flow is present. Results of a computation with a mean flow are shown.

## 6.5. Diffusion MRI

#### J.R. Li, K. V. Nguyen and I. Mekkaoui

Diffusion Magnetic Resonance Imaging (DMRI) is a promising tool to obtain useful information on microscopic structure and has been extensively applied to biological tissues. We obtained the following results.

• The Bloch-Torrey equation describes the evolution of the spin (usually water proton) magnetization under the influence of applied magnetic field gradients and is commonly used in numerical simulations for diffusion MRI and NMR. Microscopic heterogeneity inside the imaging voxel is modeled by interfaces in- side the simulation domain, where a discontinuity in the magnetization across the interfaces is produced via a permeability coefficient on the interfaces. To avoid having to simulate on a computational domain that is the size of an en- tire imaging voxel, which is often much larger than the scale of the microscopic heterogeneity as well as the mean spin diffusion displacement, smaller representative volumes of the imaging medium can be used as the simulation domain. In this case, the exterior boundaries of a representative volume either must be far away from the initial positions of the spins or suitable boundary conditions must be found to allow the movement of spins across these exterior boundaries.

Many approaches have been taken to solve the Bloch-Torrey equation but an efficient high performance computing framework is still missing. We present formulations of the interface as well as the exterior boundary conditions that are computationally efficient and suitable for arbitrary order finite elements and parallelization. In particular, the formulations use extended finite elements with weak enforcement of real (in the case of interior interfaces) and artificial (in the case of exterior boundaries) permeability conditions as well as operator splitting for the exterior boundary conditions. The method is straightforward to implement and it is available in the FEniCS for moderatescale simulations and in the FEniCS-HPC for large-scale simulations.

• 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 potentially shed light on this relationship for more complex organisms. We measured the dMRI signal of chemically-fixed abdominal ganglia of the *Aplysia* at several diffusion times. At the diffusion times measured, the dMRI signal is mono-exponential and can be accurately represented by the parameter ADC.

We analyzed the diffusion time-dependent ADC using a well-known analytical formula that is valid in the short diffusion time regime. We performed this analysis for the largest sized cells of the ganglia to satisfy the short diffusion time requirement. We noted that a naive application of the short time formula is not adequate because of the presence of the cell nucleus, making the effective cell size much smaller than the actual cell size.

We went on to perform numerical simulation of the ADC for several cell types of the abdominal ganglia. To create the simulation geometries, for the largest cells, we segmented a high resolution T2-weighted images and incorporated a manually generated nucleus. For small cells and nerve cells, we created spherical and cylindrical geometrical domains that are consistent with known information about the cellular structures from the literature. Using the library of simulation results, we fitted for the intrinsic diffusivities of the small cells and the nerve cells.

- We participated in providing simulation results for the Parietal team in their work on sensing Spindle Neurons in the Insula with Multi-shell Diffusion MRI.
- We started a new direction in the simulation and modeling of heart diffusion MRI with the postdoc project of Imen Mekkaoui, funded by Inria-EPFL lab. The project is co-supervised with Jan Hesthaven, Chair of Computational Mathematics and Simulation Science (MCSS), EPFL.

## 6.6. Mathematical tools for Psychology

#### J. R. Li and J. Hao

This is the start of a collaborative effort between the Defi team and the mental health professionals at the centre hospitalier Sainte Anne and l'Université Paris Diderot.

• We started a new research direction in algorithm and software development for analysis and classification of EEG measurements during the administration of neuropsychological tests for AD/HD with the PhD project of Jingjing Hao, co-supervised with Dr. Hassan Rahioui, Chef du pôle psychiatrique du 7e arrondissement de Paris rattaché au centre hospitalier Sainte-Anne.

## **ECUADOR Project-Team**

## 6. New Results

### 6.1. Towards Algorithmic Differentiation of C++

**Participants:** Laurent Hascoët, Benoit Dufumier, Frederic Cazals [ABS team, Inria Sophia-Antipolis], Louis Becquey [ABS team, Inria Sophia-Antipolis], Valérie Pascual.

We started the extension of Tapenade for C++. This year's first step is to connect an external C++ parser to the input formalism of Tapenade: IL. IL is an abstract language that contains the usual constructs of imperative languages. For example, the three existing parsers for Tapenade (Fortran, Fortran 95, and C) all produce Tapenade input in the form of an IL tree. Our goal was therefore to select a C++ parser or front-end and to make it produce IL trees. In parallel, our goal was also to identify the new operators, specific to Object-Oriented languages, that we must add to IL to capture C++ codes.

During their summer internship, students Benoit Dufumier from SUPELEC and Louis Becquey from INSA Lyon have drafted a C++ front-end for Tapenade, based on the tool "Clang-LLVM". They also added the new operators required into IL, and started the developments in Tapenade to manage them. At present, Tapenade is still unable to differentiate a C++ code, but it can parse and analyze a few toy C++ codes. Still, the latest release 3.13 of Tapenade does not provide any meaningful result for C++ codes yet. This work is going on.

This work benefited from the expertise in C++ of Frederic Cazals (Inria ABS team). Frederic Cazals jointly supervised both students during their internship, funded by the local Inria programme "masters transverses". The ABS team also provided the first C++ test codes and will eventually provide a large application code for Molecular Dynamics.

## 6.2. AD of mixed-language codes

Participants: Valérie Pascual, Laurent Hascoët.

The tangent differentiated code of Calculix (Three-Dimensional Structural Finite Element code), has been built and validated. Adjoint Differentiation in in progress. Driven by this application to Calculix, Tapenade is now able to differentiate mixed-language source that uses either the old style conventions or the newer Fortran 2003 primitives for interoperability with C.

Unsurprisingly, an application to such a large code uncovered a few limitations of our AD tool. One was a faulty treatment of C translation units (i.e. files), which is now fixed. C translation units or Fortran modules are two instances of the more general notion of "package" for which we need to develop more generic support in Tapenade.

### 6.3. 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 to provide reliable adjoint differentiation of C, and for our distant goal of 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, the ADMM library has been improved, and its API has been redesigned to be called from both C and Fortran. The architecture of ADMM has also been simplified, removing circular dependencies with other parts of Tapenade. The latest release 3.13 of Tapenade automatically places calls to ADMM where needed, whether the application language is C or Fortran 95. Since ADMM is a C library, the differentiated code in the Fortran case uses the Fortran 2003 standardized interoperability primitives.

In parallel, we improved the Tapenade adjoint of the "ALIF" code. ALIF 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 challenge is the intensive use of dynamic memory in ALIF, following the programming style of its model C++ code ISSM. Although successful, the usage of the ADMM library incurred some overhead. We developed a static data-flow analysis to reduce the number of calls to ADMM. This work is discussed in an article published in journal "Optimization Methods and Software"[14]

## 6.4. Application to large industrial codes

**Participants:** Valérie Pascual, Laurent Hascoët, Nicole Goutal [EDF-LNHE], Andrea Piacentini [CERFACS-GLOBC], Charlotte Kotas [Oak Ridge National Lab. (Tennessee, USA)].

We support industrial users with their first experiments of Algorithmic Differentiation of large in-house codes.

A previous collaboration with EDF and CERFACS has been continued by a new three-months contract, with the objective of improving the AD adjoint of the hydrodynamic code Mascaret. The tangent and adjoint differentiated codes have been built for the calculation of steady subcritical flow ("Sarap" kernel) with the latest Mascaret Version 8.1. The differentiation process has been simplified and it exploits the latest capacities of Tapenade on Fortran 95. In particular, the differentiated code manages Fortran 95 dynamic memory through our library ADMM. Connection with the C-written ADMM uses the Fortran 2003 standardized interoperability primitives. Validation was conducted on two test cases (named "Garonne" and "Oraison").

We support AD experiments taking place at Oak Ridge National Laboratory, targetted at building the adjoint of a large CFD application called "Rex". After one year of collaboration, we reached a first milestone with a working tangent differentiation of a sequential (i.e. non MPI) version of the code. Differentiation in tangent mode is significantly easier than in adjoint mode. Therefore it is a good practice to differentiate first in tangent mode even when the final goal is to produce gradients, which require adjoint mode. Moreover, a validated tangent code is very helpful to validate and debug an adjoint code. The next step will be extension to the MPIparallel version of the code. This will exploit and develop the AMPI library, co-developped with Argonne National Lab, for automated differentiation of MPI communication routines.

## **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 collaboration 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 most cases one order less accurate due to higher time steps and higher dissipation. For the applications to massively parallel computing, an accurate study has been undertaken in order to analyse the impact of the mesh partitioning on the parallel efficiency. Three options have been considered. The usual partition, minimizing communication under the unique constraint of uniform load over the whole domain is optimal for a part of the algorithm but performs very poorly for the other part. We have also applied the multi-constraint partitioning of Metis which relies on both whole domain balancing and fine-mesh subdomain balancing. This strategy significantly improves the efficiency, but we observed that the balancing of the whole domain phase was not perfect. A third set of experiments relied on a geometrical-based optimal multi-contraint partition which we could apply to most of our geometries and which gave a notable further improvement. An article is submitted to a journal on the basis of the second part of the thesis of Emmanuelle Itam.

### 6.6. Control of approximation errors

**Participants:** Eléonore Gauci, Alain Dervieux, Adrien Loseille [Gamma3 team, Inria-Rocquencourt], Frédéric Alauzet [Gamma3 team, Inria-Rocquencourt], Anca Belme [university of Paris 6], Gautier Brèthes [university of Montreal], Alexandre Carabias [Lemma].

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.

During this year, two works, one on the tensorial metric method started during the thesis of Gautier Brèthes [12], and one on mesh adaptation for third order approximation [13], were completed and published in journals.

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) has been submitted to a Journal.

#### **6.7. Turbulence models**

Participants: Alain Dervieux, Bruno Koobus, Stephen Wornom, Maria-Vittoria Salvetti [University of Pisa].

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 tens of millions, far too high for pure LES models. However, certain regions in the flow can be predicted better 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 models, 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.

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. 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. This model can be hybridized with a RANS model with some positive outputs. It can also be hybridized with a DDES model with larger benefits. The prediction is better than with RANS and also better than with a pure DDES model. A communication has been presented in the DLES11 conference [15] and an extended article from a conference held last year in Strasbourg has been written (with 2018 results), submitted and accepted for publication in a Springer book entitled "Progress in Hybrid RANS-LES Modelling"(2018).

## **GAMMA3** Project-Team

## 4. New Results

### 4.1. 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:

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

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:

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

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

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

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):

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

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.

## 4.2. 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).

## 4.3. 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 been 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.

## 4.4. 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.

## 4.5. 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.

## 4.6. Adaptation de maillages pour des écoulements visqueux en turbomachine

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

## 4.6.1. 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.

#### 4.6.2. 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.

#### 4.6.3. 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.

## 4.7. 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.

## 4.8. 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.

## 4.9. 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.

## 4.10. 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  $(k + 1)^{ième}$  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.

## 4.11. 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.

## 4.12. 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. Multiscale numerical methods

#### 4.1.1. Asymptotic preserving and time diminishing schemes for rarefied gas dynamic

In [10], 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 asymptotic preserving 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.

### 4.1.2. An exponential integrator for the drift-kinetic model

In [30], we propose an exponential integrator for the drift-kinetic equations in polar geometry. This approach removes the CFL condition from the linear part of the system (which is often the most stringent requirement in practice) and treats the remainder explicitly using Arakawa's finite difference scheme. The present approach is mass conservative, up to machine precision, and significantly reduces the computational effort per time step. In addition, we demonstrate the efficiency of our method by performing numerical simulations in the context of the ion temperature gradient instability. In particular, we find that our numerical method can take time steps comparable to what has been reported in the literature for the (predominantly used) splitting approach. In addition, the proposed numerical method has significant advantages with respect to conservation of energy and efficient higher order methods can be obtained easily. We demonstrate this by investigating the performance of a fourth order implementation.

## 4.1.3. Multiscale Particle-in-Cell methods and comparisons for the long-time two-dimensional Vlasov-Poisson equation with strong magnetic field

In [11], we applied different kinds of multiscale methods to numerically study the long-time Vlasov-Poisson equation with a strong magnetic field. The multiscale methods include an asymptotic preserving Runge-Kutta scheme, an exponential time differencing scheme, stroboscopic averaging method and a uniformly accurate two-scale formulation. We briefly review these methods and then adapt them to solve the Vlasov-Poisson equation under a Particle-in-Cell discretization. Extensive numerical experiments are conducted to investigate and compare the accuracy, efficiency, and long-time behavior of all the methods. The methods with the best performance under different parameter regimes are identified.

## 4.1.4. Nonlinear Geometric Optics based multiscale stochastic Galerkin methods for highly oscillatory transport equations with random inputs

In [31], we develop generalized polynomial chaos (gPC) based stochastic Galerkin (SG) methods for a class of highly oscillatory transport equations that arise in semiclassical modeling of non-adiabatic quantum dynamics. These models contain uncertainties, particularly in coefficients that correspond to the potentials of the molecular system. We first focus on a highly oscillatory scalar model with random uncertainty.

Our method is built upon the nonlinear geometrical optics (NGO) based method, developed in [12] for numerical approximations of deterministic equations, which can obtain accurate pointwise solution even without numerically resolving spatially and temporally the oscillations. With the random uncertainty, we show that such a method has oscillatory higher order derivatives in the random space, thus requires a frequency dependent discretization in the random space. We modify this method by introducing a new " time " variable based on the phase, which is shown to be non-oscillatory in the random space, based on which we develop a gPC-SG method that can capture oscillations with the frequency-independent time step, mesh size as well as the degree of polynomial chaos. A similar approach is then extended to a semiclassical surface hopping model system with a similar numerical conclusion. Various numerical examples attest that these methods indeed capture accurately the solution statistics pointwisely even though none of the numerical parameters resolve the high frequencies of the solution.

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

In [12], 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.

#### 4.1.6. 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.

## 4.1.7. A particle micro-macro decomposition based numerical scheme for collisional kinetic equations in the diffusion scaling

In [29], we derive particle schemes, based on micro-macro decomposition, for linear kinetic equations in the diffusion limit. Due to the particle approximation of the micro part, a splitting between the transport and the collision part has to be performed, and the stiffness of both these two parts prevent from uniform stability. To overcome this difficulty, the micro-macro system is reformulated into a continuous PDE whose coefficients are no longer stiff, and depend on the time step  $\Delta t$  in a consistent way. This non-stiff reformulation of the micro-macro system allows the use of standard particle approximations for the transport part, and extends a previous work where a particle approximation has been applied using a micro-macro decomposition on kinetic equations in the fluid scaling. Beyond the so-called asymptotic-preserving property which is satisfied by our schemes, they significantly reduce the inherent noise of traditional particle methods, and they have a computational cost which decreases as the system approaches the diffusion limit.

### 4.1.8. Uniformly accurate forward semi-Lagrangian methods for highly oscillatory Vlasov-Poisson equation

This work [13] is devoted to 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.

## 4.1.9. Uniformly accurate multiscale time integrators for second order oscillatory differential equations with large initial data

In [23], we apply the modulated Fourier expansion to a class of second order differential equations which consists of an oscillatory linear part and a nonoscillatory nonlinear part, with the total energy of the system possibly unbounded when the oscillation frequency grows. We comment on the difference between this model problem and the classical energy bounded oscillatory equations. Based on the expansion, we propose the multiscale time integrators to solve the ODEs under two cases: the nonlinearity is a polynomial or the frequencies in the linear part are integer multiples of a single generic frequency. The proposed schemes are explicit and efficient. The schemes have been shown from both theoretical and numerical sides to converge with a uniform second order rate for all frequencies. Comparisons with popular exponential integrators in the literature are done.

## 4.1.10. Unconditional and optimal H<sup>2</sup>-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrödinger equation in high dimensions

In [21], we focus on the optimal error bounds of two finite difference schemes for solving the *d*-dimensional (d = 2, 3) nonlinear Klein-Gordon-Schrödinger (KGS) equations. The proposed finite difference schemes not only conserve the mass and energy in the discrete level but also are efficient in practical computation because only two linear systems need to be solved at each time step. Besides the standard energy method, an induction argument as well as a 'lifting' technique are introduced to establish rigorously the optimal  $H^2$ -error estimates without any restrictions on the grid ratios, while the previous works either are not rigorous enough or often require certain restriction on the grid ratios. The convergence rates of the proposed schemes are proved to beat  $O(h^2 + \tau^2)$  with mesh size h and time step  $\tau$  in the discrete  $H^2$ -norm. The analysis method can be directly extended to other linear finite difference schemes for solving the KGS equations in high dimensions. Numerical results are reported to confirm the theoretical analysis for the proposed finite difference schemes

## 4.1.11. A combination of multiscale time integrator and two-scale formulation for the nonlinear Schrödinger equation with wave operator

In [22], we consider the nonlinear Schrödinger equation with wave operator (NLSW), which contains a dimensionless parameter  $0 < \varepsilon \leq 1$ . As  $0 < \varepsilon \ll 1$ , the solution of the NLSW propagates fast waves in time with wavelength  $O(\varepsilon^2)$  and the problem becomes highly oscillatory in time. The oscillations come from two parts. One part is from the equation and another part is from the initial data. For the ill-prepared initial data case as described in Bao and Cai (2014) which brings inconsistency in the limit regime, standard numerical methods have strong convergence order reduction in time when becomes small. We review two existing methods to solve the NLSW: an exponential integrator and a two-scale method. We comment on their order reduction issues. Then we derive a multiscale decomposition two-scale method for solving the NLSW by first performing a multiscale decomposition on the NLSW which decomposes it into a well-behaved part and an energy-unbounded part, and then applying an exponential integrator for the well-behaved part and a two-scale approach for the energy-unbounded part. Numerical experiments are conducted to test the proposed method which shows uniform second order accuracy without significant order reduction for all  $0 < \varepsilon \leq 1$ . Comparisons are made with the existing methods.

## 4.1.12. Uniformly accurate numerical schemes for the nonlinear Dirac equation in the nonrelativistic limit regime

In [18], 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  $\varepsilon$  and  $\varepsilon^2$  with epsilon  $\rightarrow 0$  in the nonrelativistic limit regime. The small parameter causes high oscillations in time which brings severe numerical burden for classical numerical methods. We transform our original problem as a two-scale formulation and present a general strategy to tackle a class of highly oscillatory problems involving the two small scales  $\varepsilon$  and  $\varepsilon^2$ . Suitable initial data for the two-scale formulation is derived to bound the time derivatives of the augmented solution. Numerical schemes with uniform (with respect to  $\varepsilon \in (0; 1]$ ) spectral accuracy in space and uniform first order or second order accuracy in time are proposed. Numerical experiments are done to confirm the UA property.

#### 4.1.13. A formal series approach to the center manifold theorem

In [6], 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.

## 4.1.14. Convergence of multi-revolution composition time-splitting methods for highly oscillatory differential equations of Schrödinger type

In [8], the convergence behaviour of multi-revolution composition methods combined with time-splitting methods is analysed for highly oscillatory linear differential equations of Schrödinger type. Numerical experiments illustrate and complement the theoretical investigations.

## 4.1.15. Highly-oscillatory evolution equations with multiple frequencies: averaging and numerics

In [7], 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.

## 4.1.16. Optimality and resonances in a class of compact finite difference schemes of high order

In [25], we revisit the old problem of compact finite difference approximations of the homogeneous Dirichlet problem in dimension 1. We design a large and natural set of schemes of arbitrary high order, and we equip this set with an algebraic structure. We give some general criteria of convergence and we apply them to obtain two new results. On the one hand, we use Padé approximant theory to construct, for each given order of consistency, the most efficient schemes and we prove their convergence. On the other hand, we use diophantine approximation theory to prove that almost all of these schemes are convergent at the same rate as the consistency order, up to some logarithmic correction.

## 4.2. mathematical analysis of multiscale partial differential equations

### 4.2.1. Collision of almost parallel vortex filaments

In [3], we investigate the occurrence of collisions in the evolution of vortex filaments through a system introduced by Klein, Majda and Damodaran and Zakharov. We first establish rigorously the existence of a pair of almost parallel vortex filaments, with opposite circulation, colliding at some point in finite time. The collision mechanism is based on the one of the self-similar solutions of the model, described in a previous

work. In the second part of this paper we extend this construction to the case of an arbitrary number of filaments, with polygonial symmetry, that are perturbations of a configuration of parallel vortex filaments forming a polygon, with or without its center, rotating with constant angular velocity.

#### 4.2.2. Free vibrations of axisymmetric shells: parabolic and elliptic cases

In [9], approximate eigenpairs (quasimodes) of axisymmetric thin elastic domains with laterally clamped boundary conditions (Lamé system) are determined by an asymptotic analysis as the thickness  $(2\varepsilon)$  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  $\varepsilon$ . Optimizing k for each chosen  $\varepsilon$ , we find power laws for k in function of  $\varepsilon$  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  $\varepsilon$  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  $\beta$ 's  $(\frac{2}{5}, \frac{3}{7}$  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.

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

In [24], the lowest eigenmode of thin axisymmetric shells is investigated for two physical models (acoustics and elasticity) as the shell thickness  $(2\varepsilon)$  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  $\varepsilon$  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  $\varepsilon$  tends to zero.

### 4.2.4. Semiclassical Sobolev constants for the electro-magnetic Robin Laplacian

This paper [15] is devoted to 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.

#### 4.2.5. On the MIT Bag Model in the Non-relativistic Limit

This paper [2] is devoted to the spectral investigation of the MIT bag model, that is, the Dirac operator on a smooth and bounded domain of  $\mathbb{R}^3$  with certain boundary conditions. When the mass m goes to  $\pm \infty$ , we provide spectral asymptotic results.

## 4.2.6. Dimension reduction for dipolar Bose-Einstein condensates in the strong interaction regime

In [4], we study dimension reduction for the three-dimensional Gross-Pitaevskii equation with a long-range and anisotropic dipole-dipole interaction modeling dipolar Bose-Einstein condensation in a strong interaction regime. The cases of disk shaped condensates (confinement from dimension three to dimension two) and cigar shaped condensates (confinement to dimension one) are analyzed. In both cases, the analysis combines averaging tools and semiclassical techniques. Asymptotic models are derived, with rates of convergence in terms of two small dimensionless parameters characterizing the strength of the confinement and the strength of the interaction between atoms.
### 4.2.7. Nonlinear stability criteria for the HMF Model

In [17], we study the nonlinear stability of a large class of inhomogeneous steady state solutions to the Hamiltonian Mean Field (HMF) model. Under a specific criterion, we prove the nonlinear stability of steady states which are decreasing functions of the microscopic energy. To achieve this task, we extend to this context the strategy based on generalized rearrangement techniques which was developed recently for the gravitational Vlasov-Poisson equation. Explicit stability inequalities are established and our analysis is able to treat non compactly supported steady states to HMF, which are physically relevant in this context but induces additional difficulties, compared to the Vlasov-Poisson system.

## 4.2.8. Strong confinement limit for the nonlinear Schrödinger equation constrained on a curve

This paper [20] is devoted to the cubic nonlinear Schrödinger equation in a two dimensional waveguide with shrinking cross section. For a Cauchy data living essentially on the first mode of the transverse Laplacian, we provide a tensorial approximation of the solution in this limit, with an estimate of the approximation error, and derive a limiting nonlinear Schrödinger equation in dimension one.

## 4.2.9. Stable ground states for the HMF Poisson Model

In [36], we prove the nonlinear orbital stability of a large class of steady states solutions to the Hamiltonian Mean Field (HMF) system with a Poisson interaction potential. These steady states are obtained as minimizers of an energy functional under one, two or infinitely many constraints. The singularity of the Poisson potential prevents from a direct run of the general strategy which was based on generalized rearrangement techniques, and which has been recently extended to the case of the usual (smooth) cosine potential. Our strategy is rather based on variational techniques. However, due to the boundedness of the space domain, our variational problems do not enjoy the usual scaling invariances which are, in general, very important in the analysis of variational problems. To replace these scaling arguments, we introduce new transformations which, although specific to our context, remain somehow in the same spirit of rearrangements tools introduced in the references above. In particular, these transformations allow for the incorporation of an arbitrary number of constraints, and yield a stability result for a large class of steady states.

### 4.2.10. The quantum Liouville-BGK equation and the moment problem

This work [19] is devoted to the analysis of the quantum Liouville-BGK equation. This equation arises in the work of Degond and Ringhofer on the derivation of quantum hydrodynamical models from first principles. Their theory consists in transposing to the quantum setting the closure strategy by entropy minimization used for kinetic equations. The starting point is the quantum Liouville-BGK equation, where the collision term is defined via a so-called quantum local equilibrium, defined as a minimizer of the quantum free energy under a local density constraint. We then address three related problems: we prove new results about the regularity of these quantum equilibria; we prove that the quantum Liouville-BGK equation admits a classical solution; and we investigate the long-time behavior of the solutions. The core of the proofs is based on a fine analysis of the properties of the minimizers of the free energy.

## 4.2.11. Averaging of nonlinear Schrödinger equations with strong magnetic confinement

In [16], 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.

## 4.3. mathematical analysis of stochastic partial differential equations

## 4.3.1. Large deviations for the dynamic $\Phi_d^{2n}$ model

In [27], we are dealing with the validity of a large deviation principle for a class of reaction-diffusion equations with polynomial non-linearity, 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  $\rho$  and  $\delta(\rho)$ , respectively, with  $0 < \rho, \delta(\rho) \ll 1$ . We prove that, under the assumption that  $\rho$  and  $\delta(\rho)$  satisfy a suitable scaling limit, a large deviation principle holds in the space of continuous trajectories with values both in the space of squareintegrable functions and in Sobolev spaces of negative exponent. Our result is valid, without any restriction on the degree of the polynomial nor on the space dimension.

#### 4.3.2. Solution to the stochastic Schrödinger equation on the full space

In [33], we show how the methods recently applied by Debussche and Weber to solve the stochastic nonlinear Schrödinger equation on  $\mathbb{T}^2$  can be enhanced to yield solutions on  $\mathbb{R}^2$  if the non-linearity is weak enough. We prove that the solutions remains localized on compact time intervals which allows us to apply energy methods on the full space.

## 4.3.3. A law of large numbers in the supremum norm for a multiscale stochastic spatial gene network

In [34], we study the asymptotic behavior of multiscale stochastic spatial gene networks. Multiscaling takes into account the difference of abundance between molecules, and captures the dynamic of rare species at a mesoscopic level. We introduce an assumption of spatial correlations for reactions involving rare species and a new law of large numbers is obtained. According to the scales, the whole system splits into two parts with different but coupled dynamics. The high scale component converges to the usual spatial model which is the solution of a partial differential equation, whereas, the low scale component converges to the usual homogeneous model which is the solution of an ordinary differential equation. Comparisons are made in the supremum norm.

## 4.3.4. Long time behavior of Gross-Pitaevskii equation at positive temperature

In [32], the stochastic Gross-Pitaevskii equation is used as a model to describe Bose-Einstein condensation at positive temperature. The equation is a complex Ginzburg Landau equation with a trapping potential and an additive space-time white noise. Two important questions for this system are the global existence of solutions in the support of the Gibbs measure, and the convergence of those solutions to the equilibrium for large time. In this paper, we give a proof of these two results in one space dimension. In order to prove the convergence to equilibrium, we use the associated purely dissipative equation as an auxiliary equation, for which the convergence may be obtained using standard techniques.

## 4.3.5. An integral inequality for the invariant measure of a stochastic reaction–diffusion equation

In [14], we consider a reaction-diffusion equation perturbed by noise (not necessarily white). We prove an integral inequality for the invariant measure  $\nu$  of a stochastic reaction-diffusion equation. Then we discuss some consequences as an integration by parts formula which extends to  $\nu$  a basic identity of the Malliavin Calculus. Finally, we prove the existence of a surface measure for a ball and a half-space of  $\mathcal{H}$ .

## 4.3.6. Kolmogorov equations and weak order analysis for SPDES with nonlinear diffusion coefficient

In [26], we provide new regularity results for the solutions of the Kolmogorov equation associated to a SPDE with nonlinear diffusion coefficients and a Burgers type nonlinearity. This generalizes previous results in the simpler cases of additive or affine noise. The basic tool is a discrete version of a two sided stochastic integral which allows a new formulation for the derivatives of these solutions. We show that this can be used to generalize the weak order analysis performed by Debussche in 2011. The tools we develop are very general and can be used to study many other examples of applications.

## 4.3.7. Approximation-diffusion in stochastically forced kinetic equations

In [35], we derive the hydrodynamic limit of a kinetic equation where the interactions in velocity are modelled by a linear operator (Fokker-Planck or Linear Boltzmann) and the force in the Vlasov term is a stochastic process with high amplitude and short-range correlation. In the scales and the regime we consider, the hydrodynamic equation is a scalar second-order stochastic partial differential equation. Compared to the deterministic case, we also observe a phenomenon of enhanced diffusion.

## **MATHERIALS Project-Team**

## 7. New Results

### 7.1. Electronic structure calculations

Participants: Éric Cancès, Virginie Ehrlacher, Antoine Levitt, Sami Siraj-Dine, 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 by an appropriate mathematical analysis, and improving the numerical approaches by a dedicated numerical analysis. We also insist on rigorously studying current materials of technological interest.

#### 7.1.1. Mathematical analysis

In [42], E. Cancès and N. Mourad performed a detailed study of the extended Kohn-Sham model for atoms subjected to cylindrically-symmetric external potentials. In particular, they computed the occupied and unoccupied energy levels of all the atoms of the first four rows of the periodic table for the reduced Hartree-Fock (rHF) and the extended Kohn-Sham  $X\alpha$  models. These results allowed them to test numerically the assumptions on the negative spectra of atomic rHF and Kohn-Sham Hamiltonians used in their previous theoretical works on density functional perturbation theory and pseudopotentials. Interestingly, they observed accidental degeneracies between s and d shells or between p and d shells at the Fermi level of some atoms.

#### 7.1.2. Numerical analysis

E. Cancès has pursued his long-term collaboration with Y. Maday (UPMC) on the numerical analysis of linear and nonlinear eigenvalue problems. Together with G. Dusson (UMPC), B. Stamm (UMPC), and M. Vohralík (Inria SERENA), they have designed a posteriori error estimates for conforming numerical approximations of the Laplace eigenvalue problem with a homogeneous Dirichlet boundary condition [15]. In particular, upper and lower bounds for any simple eigenvalue are given. These bounds are guaranteed, fully computable, and converge with the optimal speed to the exact eigenvalue. In [41], this analysis is extended to all standard numerical methods, including nonconforming discontinuous Galerkin, and mixed finite element approximations or arbitrary polynomial degree.

It is often claimed that error cancellation plays an essential role in quantum chemistry and first-principle simulation for condensed matter physics and materials science. Indeed, while the energy of a large, or even medium-size, molecular system cannot be estimated numerically within chemical accuracy (typically 1 kcal/mol or 1 mHa), it is considered that the energy difference between two configurations of the same system can be computed in practice within the desired accuracy. In [14], E. Cancès and G. Dusson initiated the quantitative study of discretization error cancellation. Discretization error is the error component due to the fact that the model used in the calculation (e.g. Kohn-Sham LDA) must be discretized in a finite basis set to be solved by a computer. They first reported comprehensive numerical simulations showing that errors on energy differences are indeed significantly smaller than errors on energies, but that these two quantities asymptotically converge at the same rate when the energy cut-off goes to infinity. They then analyzed a simple one-dimensional periodic Schrödinger equation with Dirac potentials, for which analytic solutions are available. This allowed them to explain the discretization error cancellation phenomenon on this test case with quantitative mathematical arguments.

E. Cancès, V. Ehrlacher and A. Levitt, together with D. Gontier (Dauphine) and D. Lombardi (Inria REO), have studied the convergence of properties of periodic systems as the size of the computing domain is increased. This convergence is known to be difficult in the case of metals. They have characterized the speed of convergence for a number of schemes in the metallic case, and studied the properties of a widely used numerical method that adds an artificial electronic temperature.

A. Levitt has continued his study of Wannier functions in periodic systems, after the work [16] with E. Cancès, G. Panati (Rome) and G. Stoltz was published. With H. Cornean (Aalborg), D. Gontier (Dauphine) and D. Monaco (Rome), they introduced a mathematical definition of Wannier functions for metals, used routinely in materials science but not studied theoretically until now. They proved that, under generic assumptions, there exists a set of localized Wannier functions that span a given set of bands, even if this set is not isolated from the others [50]. With A. Damle (Cornell) and L. Lin (Berkeley), they proposed an efficient numerical method for the computation of maximally-localized Wannier functions in metals, and showed on the example of the free electron gas that they are not in general exponentially localized. With D. Gontier (Dauphine) and S. Siraj-Dine, they proposed a new method for the computation of Wannier functions which applies to any insulator, and in particular to the difficult case of topological insulators.

## 7.1.3. New materials

As an external collaborator of the MURI project on 2D materials (PI: M. Luskin), E. Cancès has collaborated with P. Cazeaux (Kansas) and M. Luskin (University of Minnesota) on the computation of the electronic and optical properties of multilayer 2D materials. In particular, they have 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 [13].

The optimal design of new crystalline materials to achieve targeted electronic properties is a very important issue, in particular for photovoltaic applications. In the context of a collaboration with IRDEP, A. Bakhta (CERMICS), V. Ehrlacher and D. Gontier (Dauphine) studied the following inverse problem in [37]: given desired functions defined over the Brillouin zone of a crystalline structure, is it possible to compute a periodic potential so that the first bands of the associated periodic Schrödinger operator are as close as possible to these functions? Theoretical results were obtained for the corresponding variational problem in one dimension for the first band, and it appears from the mathematical analysis that the potential has to belong to a Borel measure space. In addition, a numerical method has been developped to solve the resulting optimization problem where the different discretization parameters are adjusted throughout the calculation, which leads to significant computational gains.

## 7.2. Computational Statistical Physics

**Participants:** Grégoire Ferré, Frédéric Legoll, Tony Lelièvre, Pierre Monmarché, Boris Nectoux, Mouad Ramil, Julien Roussel, Laura Silva Lopes, Gabriel Stoltz, Pierre Terrier.

The objective of computational statistical physics is to compute macroscopic properties of materials starting from a microscopic description of materials, using concepts of statistical physics (thermodynamic ensembles and molecular dynamics). The contributions of the team can be divided into four main topics: (i) the computation of thermodynamic quantities by sampling the canonical measure; (ii) the sampling of the stationary measure of non-equilibrium systems (namely non-reversible dynamics); (iii) the efficient computation of dynamical properties which requires to sample metastable trajectories; (iv) coarse-graining techniques to reduce the computational cost of molecular dynamic simulations and gain some insights on the models.

## 7.2.1. Sampling of the canonical measure, free energy calculations and adaptive biasing techniques

The work by T. Lelièvre and G. Stoltz, together with G. Fort (Toulouse) and B. Jourdain (CERMICS), on the study of a dynamics similar to the well-tempered metadynamics has been published [19]. This dynamics can be seen as an extension of the so-called self-healing umbrella sampling method, with a partial biasing of the dynamics only. In particular, the authors proposed a version which leads to much shorter exit times from metastable states (accelerated well-tempered metadynamics).

In [29], T. Lelièvre, in collaboration with C. Chipot (Nancy), T. Zhao, H. Fu, X. Shao, and W. Cai (Nankai University) proposed a new version of the adaptive biasing force (ABF) technique, which is well suited for the computation of free energy landscapes in high dimensions. In addition, V. Ehrlacher, T. Lelièvre and P. Monmarché are currently developping a tensorized version of the ABF algorithms. As in the usual ABF algorithm, the objective is still to compute in an adaptive way (through MCMC computations) the free energy A of a molecular system, which is a function of given reaction coordinates. To keep in memory an approximation of A requires a numerical grid of size  $m^d$  where d is the number of reaction coordinates and m is the number of points in a 1-d grid. This prevents d to be larger than 4. To allow for larger number of reaction coordinates, A is approximated as a sum of tensor products of functions of only one variable which only requires a memory of size Nmd, where N is the number of tensor products used in the approximation.

In [53], G. Stoltz and E. Vanden-Eijnden (Courant Institute) have studied the properties of the temperature accelerated molecular dynamics method. This dynamics provides a way to compute the free energy. It consists in introducing an extended variable into the system, coupled to the chosen reaction coordinate, and evolving at a higher temperature in order to alleviate metastable behavior, while the dynamics of the system at lower temperature is accelerated. G. Stoltz and E. Vanden-Eijnden proved in particular that the law of the dynamics converges exponentially fast to the steady-state, with a rate which is dictated by the Poincaré inequality of the effective dynamics on the free energy surface at higher temperature. This work was performed while E. Vanden-Eijnden was spending two months as an Inria invited professor in the project-team.

#### 7.2.2. Sampling of out-of-equilibrium dynamics

Together with A. Iacobucci and S. Olla (Univ. Dauphine), G. Stoltz studied in [20] the convergence to the steady-state of nonequilibrium Langevin dynamics, by a perturbative approach based on hypocoercive techniques developed for equilibrium Langevin dynamics. The Hamiltonian and overdamped limits (corresponding respectively to frictions going to zero or infinity) were carefully investigated. In particular, the maximal magnitude of admissible perturbations are quantified as a function of the friction. Numerical results based on a Galerkin discretization of the generator of the dynamics confirmed the relevance of the theoretical lower bounds on the spectral gap.

J. Roussel and G. Stoltz have proven the consistency of the Galerkin method for hypocoercive operators in [52]. This method allows to solve Poisson problems related to the Fokker-Planck equation very efficiently for small-dimensional systems, even if the dynamics is hypocoercive, as is the case for the Langevin dynamics for example. J. Roussel and G. Stoltz showed in particular the exponential convergence of the semigroup associated with the projected generator and provide error estimates for the solution of the numerical method, under assumptions that are proven to hold for a toy model. The authors illustrated these results by numerical experiments. In addition, an ongoing work by J. Roussel and G. Stoltz focuses on the use of control variates for non-equilibrium systems. Whereas most variance reduction methods rely on the knowledge of the invariant probability measure, this latter is not explicit out of equilibrium. Control variates offer an attractive alternative in this framework. J. Roussel and G. Stoltz proposed a general strategy for constructing an efficient control variate, relying on physical simplifications of the dynamics. The authors provide an asymptotic analysis of the variance reduction in a perturbative framework, along with extensive numerical tests on three different systems.

G. Ferré is currently working on sampling problems and rare event estimates, in particular with nonequilibrium methods. During this year, he focused on a range of methods related to the estimation of rare event probabilities, mostly based on Feynman-Kac semigroups. These processes correspond to stochastic differential equations whose trajectories are weighted, which is a form of importance sampling. This project resulted in a work on the discretization of such processes (error estimates on ergodic properties, with G. Stoltz), and led to the study of adaptive techniques, with H. Touchette (Stellenbosch). These two works will lead to publications in a close future. This research also raises questions on the long-time stability of Feynman-Kac semigroups, an issue partially covered by the litterature. G. Ferré is currently addressing this subject with G. Stoltz and M. Rousset (Inria Rennes). Other long-term projects are ongoing: one on exclusion processes with M. Simon (Inria Lille), and one on random matrices and Coulomb Gases with D. Chafai (Dauphine).

#### 7.2.3. Sampling of dynamical properties and rare events

The sampling of dynamical properties along molecular dynamics trajectories is crucial to get access to important quantities such as transition rates or reactive paths. This is difficult numerically because of the metastability of trajectories. We are following two numerical approaches to sample metastable trajectories: the accelerated dynamics  $\dot{a}$  la A.F. Voter and the adaptive multilevel splitting (AMS) technique to sample reactive paths between metastable states.

To analyze accelerated dynamics algorithms (and in particular the Temperature Accelerated Dynamics algorithm), one needs to show that the exit event from a metastable state for the Langevin or overdamped Langevin dynamics can be approximated by a kMC model parameterized by the Eyring-Kramers laws. In [45], G. Di Gesu, T. Lelièvre and B. Nectoux, together with D. Le Peutrec (Université de Paris Saclay), used the quasistationary distribution approach in order to justify the use of kinetic Monte Carlo models parameterized by the Eyring-Kramers formulas to describe exit events from metastable states. The proof is based on tools from semi-classical analysis.

Concerning the AMS technique, two recent contributions showed the interest of this approach in different applicative fields. In [51], L. Silva Lopes and T. Lelièvre analyzed the performance of the AMS method for biological systems on a simple test case: the alanine dipeptide. The interest of the method was demonstrated on this simple example: it enables to compute transition rates, to sample transition paths, and to compute reactive fluxes between two metastable states. In [26], T. Lelièvre in collaboration with H. Louvin (CEA), E. Dumonteil (IRSN), M. Rousset (Inria Rennes) and C.M. Diop (CEA) implemented the AMS method in the framework of nuclear safety. The idea was to use the AMS method to compute neutron fluxes in strongly absorbing media, for shielding applications. The method has been implemented in Tripoli 4, and gives very interesting results compared to the classical exponential biasing approach, in particular for neutron branching processes.

#### 7.2.4. Coarse-graining

In [25], F. Legoll and T. Lelièvre, in collaboration with S. Olla (Dauphine), analyzed 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*. More precisely, a pathwise error estimate was obtained, which is an improvement compared to a previous result by F. Legoll and T. Lelièvre where only the marginal in times were considered. This analysis is also useful to obtain quantitative estimate for some averaging procedure on two-scale dynamics.

G. Stoltz developed new numerical methods to stabilize the time discretization of generalizations of Langevin dynamics, more precisely dissipative particle dynamics with energy conservation (DPDE) and smoothed dissipative particle dynamics (SDPD). The latter case was studied with a PhD student, Gérôme Faure (CEA/DAM and CERMICS). These two models describe mesoscopic systems of particles with two global invariants: energy and momentum. The numerical schemes are obtained as the composition of a Verlet integration of the deterministic part of the dynamics, and successive integration of the pairwise fluctuation-dissipation dynamics. These elementary dynamics are the one which need to be stabilized because too large timesteps can lead to negative internal energies of the particles. The idea of the methods is to rewrite the elementary 8-dimensional fluctuation-dissipation dynamics as effective reversible one-dimensional dynamics on the relative velocities, which can then be Metropolized; see [27] for DPDE and [18] for SDPD.

In [28], a joint work with Manuel Athènes, Thomas Jourdan (CEA/Saclay SRMP) and Gilles Adjanor (EDF R&D, MMC), G. Stoltz and P. Terrier presented a coupling algorithm for cluster dynamics. 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 equations. Nevertheless this approach is still limited by the number of equations to solve in the case of complex materials. Fully stochastic simulations see the RECD as a master equation, hence reducing

the number of equations to solve to the number of stochastic particles, but are limited by the high frequency of certain events. The proposed algorithm is based on a splitting of the dynamics and combines deterministic and stochastic approaches. It is generic (allowing different stochastic approaches such as a jump process or a Langevin dynamics based on the Fokker-Planck approximation) and is highly parallelizable. The accuracy of this new algorithm is illustrated in a case of vacancy clustering of materials under thermal ageing. Numerical analysis of the algorithm shows that the errors due to the splitting (a standard Lie-Trotter splitting) and due to the stochastic approaches decrease according to the theory, *i.e.* respectively linearly with the time step and as  $N^{-1/2}$ , N being the number of stochastic particles. The error due to the Fokker-Planck approximation is currently under study.

## 7.3. Homogenization

**Participants:** Virginie Ehrlacher, Marc Josien, Claude Le Bris, Frédéric Legoll, Adrien Lesage, Pierre-Loïk Rothé.

#### 7.3.1. Deterministic non-periodic systems

In homogenization theory, members of the project-team have pursued their systematic study of perturbations of periodic problems (by local and nonlocal defects). This has been done in two different directions. For linear elliptic equations, they have first, in collaboration with X. Blanc (Paris Diderot) and P-L. Lions (Collège de France), provided a more versatile proof on local defects, and also extended their analysis to advection-diffusion equations. Second, they have also provided more details on the quality of approximation achieved by their theory. These are works in preparation with X. Blanc and M. Josien (Matherials). On the other hand, they have approached the same perturbation problem but for nonlinear equations. The specific case considered is that of viscosity solutions of Hamilton-Jacobi equations, and the work has been completed in collaboration with Pierre Cardaliaguet (Paris Dauphine) and Panagiotis Souganidis (University of Chicago), see [43]. To the best knowledge of the authors, this is the first time such a perturbation has been studied for this type of nonlinear equations.

#### 7.3.2. Stochastic homogenization

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

In addition, a question of interest is to describe how the oscillatory solution  $u_{\epsilon}$  fluctuates around its effective behavior (which is given by the homogenized limit  $u^*$ ). This question is investigated in the PhD thesis of P.-L. Rothé. Results have been obtained for a weakly stochastic framework (with a periodic coefficient and a small random perturbation). It has been shown that, at the first order, the fluctuations are at the scale  $\epsilon^{-\frac{d}{2}}$ . Furthermore when  $\epsilon$  is small, the localized fluctuations (characterized by a test function g) of  $u_{\epsilon}$  are Gaussian. The corresponding variance depends on the localization function g and on a fourth order tensor Q. A numerical approach has been designed to approximate Q and its convergence has been proven. Numerical experiments in more general settings (full stochastic case) following the same approach have been performed. The results are promising.

#### 7.3.3. 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.

During the year, the final writing of the various works performed in the context of the PhD thesis of F. Madiot has been completed. The comparison of the various MsFEM approaches has been documented in [24]. The case of an advection-diffusion equation with a dominating convection in a perforated domain is completely studied in [47]. For the latter equation, the approach based on the introduction of the invariant measure has been described, tested and studied in [48].

One of the perspectives of the team, through the thesis of A. Lesage, is the development of a multiscale finite element method for thin heterogeneous plates. The fact that one of the dimension of the domain of interest scales typically like the typical size of the heterogeneities within the material induces theoretical and practical difficulties that have to be carefully taken into account.

## 7.3.4. Dislocations

In the context of the PhD thesis of M. Josien, some results have been obtained regarding the modeling and numerical simulation of 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. the Weertman equation and the dynamical Peierls-Nabarro equation), involving non-local operators.

In collaboration with C. Le Bris, F. Legoll and Y.-P. Pellegrini (CEA-DAM), M. Josien has first focused on the steady state regime (the Weertman equation), and has designed a numerical method for approximating its solution. This relies on a preconditioned scheme based on a dynamical system that integrates differently the linear nonlocal terms (by means of the Fourier transform) and the nonlinear local terms. The numerical scheme is described in [21]. M. Josien has mathematically studied the Weertman equation. In particular, under physically relevant hypotheses, it has been shown in [46] that the equation is the long-term limit of a dynamical system, namely exactly that which has been used for the numerical approximation. The time-dependent regime of a dislocation involves an integrodifferential equation with memory kernel (the so-called Dynamic Peierls-Nabarro equation). M. Josien is currently working on possible numerical approaches to solve it, and is writing a code that is intended to be used in some simple physical test cases. A special effort is devoted to the memory aspect of this equation, using techniques designed by Ch. Lubich and collaborators.

## 7.4. Complex fluids

Participants: Sébastien Boyaval, Dena Kazerani.

The aim of the research performed in the project-team about complex fluids is

- to guide the mathematical modeling with PDEs of multi-phase flowing materials, like liquid suspensions of particles or stratified air-water flows, and
- to propose efficient algorithms for the computation of flow solutions, mainly for the many applications in the hydraulic engineering context.

The analysis of heterogeneous flow models for the paradigmatic complex fluids of Maxwell type has been pursued [38], [34], in particular for gravity flows with a free surface (natural in the hydraulic engineering context). It is planned to pursue the analysis with other fluids, and obtain thereby mathematically-sound models for the erosion of sediment. Dena Kazerani has recently started working on that goal, in the context of the on-going ANR JCJC project SEDIFLO of S. Boyaval with E. Audusse (Paris 13), A. Caboussat (Genève), A. Lemaitre (ENPC) and M. Parisot (Inria ANGE).

Even for Newtonian fluids like water, the simpler models that are currently used do not always produce satisfactory numerical results in the hydraulic engineering context, especially because the data that is used to perform numerical predictions is uncertain. Considering that some model uncertainties induce (stochastic) parametric variations like material heterogeneities, S. Boyaval pursued his analysis of new fast algorithms to compute many PDE solutions for many parameter values in the (uncertain) hydraulic engineering context [30], [54].

## 7.5. Various topics

### Participant: Virginie Ehrlacher.

In the context of a collaboration with EDF, V. Ehrlacher, together with A. Benaceur, A. Ern (CERMICS) and S. Meunier (EDF) has developed in [35] a new reduced basis methodology for parabolic nonlinear systems of equations which enables to significantly reduce the computational time of the offline phase of the method.

V. Ehrlacher, with T. Boiveau, A. Ern (CERMICS) and A. Nouy (Centrale Nantes), has developed a new global space-time unconditionally stable approximation scheme for linear parabolic equations, which relies on the Lions-Magenes formulation of such partial differential equations, in [39]. Such a formulation is perfectly adapted for the use of tensor methods to approximate the solution of these equations at a significantly lower computational cost, based on the separation of space and time variables. Different greedy algorithms to compute this tensor approximation of the solution are compared on numerical testcases using several formulations including the new proposed one. The new approach enables to define a provably convergent algorithm with better approximation properties than the other methods.

## **MEMPHIS Project-Team**

## 7. New Results

## 7.1. Fluid-structure interaction and a monolithic scheme

Fluid-structure interaction (FSI) problems are still today difficult to solve on the numerical point of view. Memphis team works on the development of a new numerical method for the simulation of these phenomenas. This method relies on a FSI coupling scheme called "monolithic", in which an eulerian hyperelastic model (Mooney-Rivlin) predicts the behaviour of an elastic structure, all of this in the context of an implicit inclusion of the geometry. A 2D axi-symmetric incompressible Navier-Stokes model is used to follow the behaviour of a newtonian fluid, interacting with this elastic body.

With this coupling method, the solid and fluid problems are solve as a unique numerical solver. This approach has already been studied in the Memphis team for compressible fluids. This process seems to be interesting while it competes on the accuracy point of view with the partitioned approches, commonly used in the literature. More over, an eulerian formalism releases us from the constraints related to the tracking of the fluid-structure interface, which remains the key difficulty for lagrangian methods. This implicit consideration is therefore coherent from the perspective of including complexe geometries. In responding to difficulties related to the monolithic scheme, we employ a kind of meshing, particularly adapted to AMR (Adaptative Mesh Refinement). Developed by the OPTIMAD society, the library PABLO offers the ability to build conceptually simple meshes, natively parallel, and convenient to use. The hierarchical cartesian meshes are also particularly adapted to complex geometries.

The fluid-structure interface is followed via a level-set function. This one is transported in time with a 2nd order semi-lagrangian scheme which is volume conservative, and it is frequently reinitialize with a redistanciation algorithm. A linear extrapolation algorithm (Aslam) is besides added as a complement to the elastic model in order to limit the "non physical" effects introduced by the monolithic coupling scheme. Finally, a contact model is employed to model the collision between an elastic solid and a rigid solid which can occur in particular in a cardiac pump based on oscillating membranes.



*Figure 8. Two FSI problems. On the left: elastic cylinder colliding a rigid plate; on the right: hyperelastic membrane immersed in a pump geometry, moving thanks to a mechanical oscillating actuator.* 

## 7.2. A Local Lubrication Model for Spherical Particles within an Incompressible Navier-Stokes Flow

The lubrication effects are short-range hydrodynamic interactions essential to the suspension of the particles, and are usually underestimated by direct numerical simulations of particle laden flows.

A local lubrication correction model for particle laden flow of spherical solid particles has been presented and validated. Interactions between a particle and an obstacle (another particle or a wall) can be decomposed into three types: long range hydrodynamics, short range hydrodynamics also called lubrication effects, and mechanical solid-solid contacts.

Long range hydrodynamic interaction are fully resolved by the Volume Penalization method (VP). The incompressible Navier-Stokes equations have been discretized in time using a scalar projection method and in space with a fully second order penalty method.

Due to unresolved scales associated with the grid, short range hydrodynamic interactions are only partially captured by the numerical approach. We thus introduce a local lubrication model. This correction is based on asymptotic expansions of analytical solutions of particle-particle or particle-wall interactions, assuming that the flow within the gap between the particle and the obstacle is in the Stokes regime. Lubrication forces and torques are corrected in a neighborhood of the contact point of two interacting particles where lubrication is poorly captured, as long as the normalized gap width  $\epsilon$  is smaller than a critical length  $\epsilon_{lub}$  (a model parameter).

Finally, a linear soft-sphere collision model is used for solid-solid contacts. This model, widely used in the literature [Costa15,Izard14], represents mechanical contacts as two spring-dashpot systems connected at the contact point. The model allows stretching the collision time, to avoid computational overhead in the calculation of the collision force, making the method particularly efficient.

Our local lubrication correction model have been validated on several benchmarks. First, we considered a single particle falling onto a wall at various approach velocities. The comparison with experimental results [Harada01,Joseph01] enables us to validate the dominant lubrication component resulting from the squeezing of the fluid in the gap. The lubrication force and the torque created by the shearing of the fluid in the gap have been validated on oblique particle-wall collisions in dry and wet systems proposed by Joseph and Hunt [Joseph04]. Since lubrication corrections are made locally, our lubrication model does not required tabulation and is compatible to non-spherical particles. The model will be tested for polydisperse flow of ellipsoidal particles in future works.

## 7.3. Incompressible flow schemes on octrees.

The incompressible Navier-Stokes solver was validated in 2D last years thanks to the computation of the order of convergence. This year, a comparison has been done with data from literature. A first test-case was the flow around a 2-D cylinder. On the figure 9 can be seen a comparison between results from the developed solver and data from literature [Ploumhans (2000)].

A second test case was the flow around a Naca0012 airfoil. The figure 10 shows the X-Velocity around the airfoil at Re = 1000 with an angle of attack of 15°. A QuadTree grid has been used as can be seen in figure 11 . The aerodynamic coefficients have been computed for this test-case and have been compared with data from literature [D. F. Kurtulus (2015)]. With  $C_D mean = 0.3$  and  $C_L mean = 0.6$  the results are in good agreement with  $C_D mean = 0.3$  and  $C_L mean = 0.7$  from literature data gathered in [D. F. Kurtulus (2015)].

Then, a grid adaptation process has been developed. It allows for exemple to deal with moving bodies and to focus on interesting areas in the computational domain. With user defined criteria, the grid is indeed automatically refined or coarsened. So, this code allows a fast meshing of the computational domain thanks to the penalization approach. An interesting compromise between computational time and accuracy is also reached thanks to the adaptive mesh refinement process. A validation of the adaptive mesh refinement process has been done with a comparison between 2 cases : the case of the flow around a fixed body with an inflow of  $1m.s^{-1}$  and the case of a moving body with a velocity of  $1m.s^{-1}$  in a fixed flow. It can be seen on figure 12.

An extension of the code to 3-D has been developed and validated. Again, 2 different test-cases has been chosen for the validation. First, the flow around a sphere has been computed at different Reynolds number and a comparison has been done with several data from literature as shown in table 1. The figure 13 shows the X-Velocity of the flow around a sphere at Re = 500 with Octree grid. A LES turbulence model has been implemented with a Vreman subgrid model. So, the second test-case is the flow around a cylinder at



Figure 9. Comparison of drag coefficients between the code developped and data from literature for the flow around a cylinder at Re = 550



Figure 10. X-Velocity around a Naca0012 airfoil at Re = 1000 with an angle of attack of  $15^{\circ}$ 



Figure 11. QuadTree grid around a Naca0012 airfoil



Figure 12. Comparison with drag coeficient obtained with a fixed body in a flow and with a moving body with a velocity of  $1m.s^{-1}$  in a fixed flow

Re = 3900 with LES. The wake profile at different positions has been compared with experimental data as can be seen in figure 14.

Re	Present work	[Campregher	[Fornberg	[Fadlun et al.	[Kim et al.	[Subramanian
		(2009)]	(1988)]	(2000)]	(2001)]	(2003)]
300	0.6268	0.675	-	-	0.657	0.653
500	0.5488	0.52	0.4818	0.476	-	0.555

Table 1. Comparison of drag coefficients with data from literature at different Reynolds Number



*Figure 13. X-Velocity around a sphere at* Re = 500

As the overall aim is to simulate the aeroelastic effects on a wind turbine subjected to gusts, a dynamic beam model with axial, torsional and flexural deformations have been implemented and coupled with the Octree Navier-Stokes solver.

# 7.4. Validation of NaSCar at higher Reynolds numbers and Aeroelastic coupling

A beam finite element model has been implemented in order to study the dynamic behavior of the wind turbine blade. The structural model is linear and can describe bending, torsion and axial deformation. There is the possibility to take into account some coupling effects between bending-torsion and torsion-axial deformation. The implementation of the structural model has been validated by means of different static and dynamic tests. In **15** the Fast Fourier Transform of the tip deflection history is reported: the frequency of the predicted peaks is in good agreement with the theoretical values.

The structural model has been coupled with two different computational fluid dynamics codes: a cartesian code (NASCAR3d) and an octree code (developed by Claire Taymans during her PhD). The coupling requires to compute the loads for the structural model by performing an integral of the fluid forces on a surface mesh. The surface mesh is updated at each time step according to the displacement of the structure and this allows to update the level set which is used to impose the effects of the body on the fluid.

51



Figure 14. Wake profile at different positions behind a cylinder at Re = 3900 obtained by averaging Velocity after a preliminary simulation



Figure 15. spectrum of the tip deflection

In order to focus the attention on a single blade of the rotor, the inertial terms (centrifugal and Coriolis forces) have been added in both the fluid solver and in the structural model. This makes it possible to perform a preliminary study of the behavior of a single elastic blade by neglecting the interactions between the different blades and the wind turbine's tower (see 16).



Figure 16. velocity vector field and q-criterion vorticity contour around the turbine blade

The turbulent flow around the blade is studied by means of the Vreman Large Eddy Simulation model  $^{0}$  which has been tested on the flow around a cylinder at Re=3900 and Re=140000. The validation of the model for high reynolds flows required the use of a very fine mesh in order to appropriately simulate turbulent disspation and accurately predict the mean flow field, the results obtained are in good agreement with the experimental data of Cantwell et al  $^{0}$ , as reported in 17.



Figure 17. Cylinder mean wake velocity profiles, Re=140000

<sup>&</sup>lt;sup>0</sup>A.W. Vreman, "'An eddy-viscosity subgrid-scale model for turbulent shear flow: Algebraic theory and applications,"' Phys. Fluids 16,10 (2004)

<sup>&</sup>lt;sup>0</sup>B. Cantwell, D. Coles, "'An experimental study of entrainment and transport in the turbulent near wake of a circular cylinder,"' J. Fluid Mech. (1983), vol. 136, pp. 321-374

In order to extend the capability of the code to high Reynolds number a wall function approach has been implemented following the guidelines of De Tullio<sup>0</sup>. The main idea of this approach is to impose the value of the velocity in the first fluid cells close to the wall by performing a non-linear interpolation based on wall function which represents the velocity distribution in the turbulent boundary layer (see 18).



Figure 18. wall correction

## 7.5. Thoracic implant

We are interested in the simulation of elastic tissus deformation in order to simulate the skin deformation due to the pose of a thoracic implant. These implants are used to fill the sternum cavity of patients affected by Pectus Excavatum syndrom. As a first step, we simulated the skin deformation with a single layer elastic model from the real bones, skin and implant geometries imported from STL files. The implant geometry has been designed on-demand by Anatomik Modeling. The single layer elastic model representing an underskin implant, has been implemented on an octree grid to easily and automatically refine around the different geometries and keep accuracy.

The results obtained were qualitatively validated by Anatomik Modeling. The implant actually lays on the rib cage, under the muscles. The next step will be then to include a multi-layer elasticity model to take into account the muscles and other biological soft tissus.

Another problem linked to custom made thoracic implants is the extraction of the so-called surgical plan. It is a critical step necessary to design the implant. This plan corresponds to the surface of the rib cage. To extract it, a mass-spring model has been developed and integrated in a software prototype with a graphical interface. The resulting prototype can be used easily from on any rib cage described by a STL file.

<sup>&</sup>lt;sup>0</sup>De Tullio, M.D. (2006) *Development of an Immersed Boundary method for the solution of the preconditioned Navier-Stokes equations* (PhD thesis)



Figure 19. Left: Automatic refinement around a part of the rib cage. Right: Slice of the signed distance fonction from rib cage and skin with automatic refinement





Figure 20. Left: Skin without implant. Right: Skin simulation with implant under skin

## **MEPHYSTO Project-Team**

## 4. New Results

## 4.1. Long-time homogenization of the wave equation

In a joint work [36], A. Benoit and A. Gloria considered an elliptic operator in divergence form with symmetric coefficients. If the diffusion coefficients are periodic, the Bloch theorem allows one to diagonalize the elliptic operator, which is key to the spectral properties of the elliptic operator and the usual starting point for the study of its long-time homogenization. When the coefficients are not periodic (say, quasi-periodic, almost periodic, or random with decaying correlations at infinity), the Bloch theorem does not hold and both the spectral properties and the long-time behavior of the associated operator are unclear. At low frequencies, we may however consider a formal Taylor expansion of Bloch waves (whether they exist or not) based on correctors in elliptic homogenization. The associated Taylor-Bloch waves diagonalize the elliptic operator up to an error term (an "eigendefect"), which we express with the help of a new family of extended correctors. We use the Taylor-Bloch waves equation in terms of the spatial growth of these extended correctors. On the one hand, this quantifies the validity of homogenization over large times (both for the standard homogenized equation and higher-order versions). On the other hand, this allows us to prove asymptotic ballistic transport of classical waves at low energies for almost periodic and random operators.

## 4.2. Weighted functional inequalities

Functional inequalities like spectral gap, covariance, or logarithmic Sobolev inequalities are powerful tools to prove nonlinear concentration of measure properties and central limit theorem scalings. Besides their well-known applications in mathematical physics (e.g. for the study of interacting particle systems like the Ising model or for interface models), such inequalities were recently used by the team to establish quantitative stochastic homogenization results.

These functional inequalities have nevertheless two main limitations for stochastic homogenization. On the one hand, whereas only few examples are known to satisfy them (besides product measures, Gaussian measures, and more general Gibbs measures with nicely behaved Hamiltonians), these inequalities are not robust with respect to various simple constructions: for instance, a Poisson point process satisfies a spectral gap, but the random field corresponding to the Voronoi tessellation of a Poisson point process does not. On the other hand, these functional inequalities require random fields to have an integrable covariance, which prevents one to consider fields with heavier tails.

In the series of work [26], [27], [28], M. Duerinckx and A. Gloria introduced weaker versions of these functional inequalities in the form of weighted inequalities. The interest of such inequalities is twofold: first, as their unweighted counterpart they ensure strong concentration properties; second, they hold for a large class of statistics of interest to homogenization (which is shown using a constructive approach).

## 4.3. Macroscopic behaviors of large interacting particle systems

A vast amount of physical phenomena were first described at the macroscopic scale, in terms of the classical partial differential equations (PDEs) of mathematical physics. Over the last decades the scientific community has pursued part of its research towards the following *universality principle*, which is well known in statistical physics: "the qualitative behavior of physical systems depend on the microscopic details of the system only through some large-scale variables". Typically, the microscopic systems are composed of a huge number of atoms and one looks at a very large time scale with respect to the typical frequency of atom vibrations. Mathematically, this corresponds to a space-time scaling limit procedure.

The macroscopic laws that can arise from microscopic systems can either be partial differential equations (PDEs) or stochastic PDEs (SPDEs) depending on whether one is looking at the convergence to the mean or at the fluctuations around that mean. Therefore, it is a natural problem in the field of interacting particle systems to obtain the macroscopic laws of the relevant thermodynamical quantities, using an underlying microscopic dynamics, namely particles that move according to some prescribed stochastic law. Probabilistically speaking, these systems are continuous time Markov processes.

### 4.3.1. Anomalous diffusion

First, one can imagine that at the *microscopic* scale, the population is well modeled by stochastic differential equations (SDEs). Then, the *macroscopic* description of the population densities is provided by partial differential equations (PDEs), which can be of different types. All these systems may characterize the collective behavior of individuals in biology models, but also agents in economics and finance. In [14] M. Simon in collaboration with C. Olivera has obtained a limit process which belongs to the family of non-local PDEs, and is related to anomalous diffusions. More precisely, they study the asymptotic behavior of a system of particles which interact *moderately*, i.e. an intermediate situation between weak and strong interaction, and which are submitted to random scattering. They prove a law of large numbers for the empirical density process, which in the macroscopic limit follows a fractional conservation law. The latter is a generalization of convection-diffusion equations, and can appear in physical models (e.g. over-driven detonation in gases [38], or semiconductor growth [55]), but also in areas like hydrodynamics and molecular biology.

Another approach which aims at understanding this abnormally diffusive phenomena is to start from deterministic system of Newtonian particles, and then perturb this system with a stochastic component which will provide enough ergodicity to the dynamics. It is already well known that these stochastic chains model correctly the behavior of the conductivity [35]. In two published papers [18][32], and another submitted one [19], M. Simon with her coauthors C. Bernardin, P. Gonçalves, M. Jara, T. Komorowski, S. Olla and M. Sasada have observed both behaviors, normal and anomalous diffusion, in the context of low dimensional asymmetric systems. They manage to describe the microscopic phenomena at play which are responsible for each one of these phenomena, and they go beyond the predictions that have recently been done in [51], [52].

### 4.3.2. Towards the weak KPZ universality conjecture

Among the classical SPDEs is the Kardar-Parisi-Zhang (KPZ) equation which has been first introduced more than thirty years ago in [46] as the *universal* law describing the fluctuations of randomly growing interfaces of one-dimensional stochastic dynamics close to a stationary state (as for example, models of bacterial growth, or fire propagation). In particular, the weak KPZ universality conjecture [52] states that the fluctuations of a large class of one-dimensional microscopic interface growth models are ruled at the macroscopic scale by solutions of the KPZ equation. Thanks to the recent result of M. Jara and P. Gonçalves [45], one has now all in hands to establish that conjecture. In their 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 [13], M. Simon in collaboration with P. Gonçalves and M. Jara give a new proof of that principle, which does not impose the knowledge on the spectral gap inequality for the underlying model and relies on a proper decomposition of the antisymmetric part of the current of the system in terms of polynomial functions. In addition, they fully derive the convergence of the equilibrium fluctuations towards (1) a trivial process in case of super-diffusive systems, (2) an Ornstein-Uhlenbeck process or the unique energy solution of the stochastic Burgers equation (SBE) (and its companion, the KPZ equation), in case of weakly asymmetric diffusive systems. Examples and applications are presented for weakly and partial asymmetric exclusion processes, weakly asymmetric speed change exclusion processes and Hamiltonian systems with exponential interactions.

In [30], M. Simon together with P. Gonçalves and N. Perkowski go beyond the weak KPZ universality conjecture to derive a new SPDE, namely, the KPZ equation with boundary conditions, from an interacting particle system in contact with stochastic reservoirs. They legitimate the choice done at the macroscopic level for the KPZ/SBE equation from the microscopic description of the system. For that purpose, they prove two main theorems: first, they extend the notion of energy solutions to the stochastic Burgers equation

by adding Dirichlet boundary conditions. Second, they construct a microscopic model (based on weakly asymmetric exclusion processes) from which the energy solution naturally emerges as the macroscopic limit of its stationary density fluctuations. This gives a physical justification for the Dirichlet boundary conditions the SBE equation. They also prove existence and uniqueness of energy solutions to two related SPDEs: the KPZ equation with Neumann boundary conditions and the SHE with Robin boundary conditions, and they rigorously establish the formal links between the equations. This is more subtle than expected, because the boundary conditions do not behave canonically. Finally, they associate an interface growth model to the microscopic model, roughly speaking by integrating it in the space variable, and show that it converges to the energy solution of the KPZ equation, thereby giving a physical justification of the Neumann boundary conditions.

# 4.4. High order exponential integrators for nonlinear Schrödinger equations with application to rotating Bose–Einstein condensates

In a recent work with C. Besse and I. Violet [6], Guillaume Dujardin has proposed and analyzed new methods for the time integration of the nonlinear Schrödinger equation in the context of rotating Bose–Einstein condensates. In particular, he has proposed a systematic way to design high-order in time implicit exponential methods, given sufficient conditions to ensure mass preservation by the methods and proved high order in several physically relevant situations. He has compared those methods to several other popular methods from the literature and provided several numerical experiments.

# 4.5. Periodic modulations controlling Kuznetsov-Ma soliton formation in nonlinear Schrödinger equations

Together with colleages from the Physics department of the Université de Lille, S. de Bièvre and G. Dujardin have analyzed the exact Kuznetsov–Ma soliton solution of the one-dimensional nonlinear Schrödinger equation in the presence of periodic modulations satisfying an integrability condition [15]. They showed that, in contrast to the case without modulation, the Kuznetsov–Ma soliton develops multiple compression points whose number, shape and position are controlled both by the intensity of the modulation and by its frequency. In addition, when this modulation frequency is a rational multiple of the natural frequency of the Kuzzetsov–Ma soliton's intensity are periodic. When the ratio of the two frequencies is irrational, the soliton's intensity is a quasiperiodic function. A striking and important result of this analysis is the possibility to suppress any component of the output spectrum of the Kuznetsov–Ma soliton by a judicious choice of the amplitude and frequency of the modulation.

# 4.6. Exponential integrators for nonlinear Schrödinger equations with white noise dispersion

Together with D. Cohen, G. Dujardin has proposed several exponential numerical methods for the time integration of the nonlinear Schrödinger equation with power law nonlinearity and random dispersion [11]. In particular, he introduced a new explicit exponential integrator for this purpose that integrates the noisy part of the equation exactly. He prove that this scheme is of mean-square order 1 and he drew consequences of this fact. He compared the exponential integrator with several other numerical methods from the literature. Finally, he proposed a second exponential integrator, which is implicit and symmetric and, in contrast to the first one, preserves the  $L^2$ -norm of the solution.

## 4.7. New results on waveguides with mixed diffusion

In [21], [8], [22], D. Bonheure, J.-B. Casteras and collaborators obtained new results on the existence and qualitative properties of waveguides for a mixed-diffusion NLS equation. In particular, they proved the first existence results for waveguides with fixed mass and provided several qualitative descriptions of these. They also showed that the ground-state solutions are instable by finite (or infinite) time blow-up improving a recent result of Boulenger and Lenzmann and answering a conjecture of Baruch and Fibich.

## 4.8. New result on the Boltzmann scenario

Boltzmann provided a scenario to explain why individual macroscopic systems inevitably approach a unique macroscopic state of thermodynamic equilibrium, and why after having done so, they remain in that state, apparently forever. In [12], new rigorous results are provided that mathematically prove the basic features of Boltzmann's scenario for two classical models: a simple boundary-free model for the spatial homogenization of a non-interacting gas of point particles, and the well-known Kac ring model.

## 4.9. Other new results

In [9], [20], D. Bonheure, J.-B. Casteras and collaborators made bifurcation analysis and constructed multilayer 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 [10], [23], J.-B. Casteras and collaborators study different problems related to the existence of A-harmonic functions with prescribed asymptotic boundary on Cartan-Hadamard manifold. In particular, they obtained a sharp lower bound on the section curvature for the existence of minimal graphic functions with prescribed asymptotic boundary.

In [25], a kinetic equation of the Vlasov-Wave type is studied, which arises in the description of the behavior of a large number of particles interacting weakly with an environment. Variational techniques are used to establish the existence of large families of stationary states for this system, and analyze their stability.

## **MOKAPLAN Project-Team**

## 6. New Results

## 6.1. Optimal transport for diffeomorphic registration

J. Feydy and B. Charlier and G. Peyré and F-X. Vialard

[18]

This paper introduces the use of unbalanced optimal transport methods as a similarity measure for diffeomorphic matching of imaging data. The similarity measure is a key object in diffeomorphic registration methods that, together with the regularization on the deformation, defines the optimal deformation. Most often, these similarity measures are local or non local but simple enough to be computationally fast. We build on recent theoretical and numerical advances in optimal transport to propose fast and global similarity measures that can be used on surfaces or volumetric imaging data. This new similarity measure is computed using a fast generalized Sinkhorn algorithm. We apply this new metric in the LDDMM framework on synthetic and real data, fibres bundles and surfaces and show that better matching results are obtained.

## 6.2. Quantum Optimal Transport for Tensor Field Processing

G. Peyré and L. Chizat and F-X. Vialard and J. Solomon

[18]

This article introduces a new notion of optimal transport (OT) between tensor fields, which are measures whose values are positive semidefinite (PSD) matrices. This "quantum" formulation of OT (Q-OT) corresponds to a relaxed version of the classical Kantorovich transport problem, where the fidelity between the input PSD-valued measures is captured using the geometry of the Von-Neumann quantum entropy. We propose a quantum-entropic regularization of the resulting convex optimization problem, which can be solved efficiently using an iterative scaling algorithm. This method is a generalization of the celebrated Sinkhorn algorithm to the quantum setting of PSD matrices. We extend this formulation and the quantum Sinkhorn algorithm to compute barycenters within a collection of input tensor fields. We illustrate the usefulness of the proposed approach on applications to procedural noise generation, anisotropic meshing, diffusion tensor imaging and spectral texture synthesis.

# 6.3. The Camassa-Holm equation as an incompressible Euler equation: a geometric point of view

### T. Gallouët and F-X. Vialard

#### [35]

The group of diffeomorphisms of a compact manifold endowed with the L2 metric acting on the space of probability densities gives a unifying framework for the incompressible Euler equation and the theory of optimal mass transport. Recently, several authors have extended optimal transport to the space of positive Radon measures where the Wasserstein-Fisher-Rao distance is a natural extension of the classical L2-Wasserstein distance. In this paper, we show a similar relation between this unbalanced optimal transport problem and the Hdiv right-invariant metric on the group of diffeomorphisms, which corresponds to the Camassa-Holm (CH) equation in one dimension. On the optimal transport side, we prove a polar factorization theorem on the automorphism group of half-densities.Geometrically, our point of view provides an isometric embedding of the group of diffeomorphisms endowed with this right-invariant metric in the automorphisms group of the fiber bundle of half densities endowed with an L2 type of cone metric. This leads to a new formulation of the (generalized) CH equation as a geodesic equation on an isotropy subgroup of this

automorphisms group; On S1, solutions to the standard CH thus give particular solutions of the incompressible Euler equation on a group of homeomorphisms of R2 which preserve a radial density that has a singularity at 0. An other application consists in proving that smooth solutions of the Euler-Arnold equation for the Hdiv right-invariant metric are length minimizing geodesics for sufficiently short times.

# 6.4. Minimal convex extensions and finite difference discretization of the quadratic Monge-Kantorovich problem

J-D. Benamou and V. Duval

[25]

We designed an adaptation of the MA-LBR scheme [4] to the Monge-Ampère equation with second boundary value condition, provided the target is a convex set. This yields a fast adaptive method to numerically solve the Optimal Transport problem between two absolutely continuous measures, the second of which has convex support. The proposed numerical method actually captures a specific Brenier solution which is minimal in some sense. We prove the convergence of the method as the grid stepsize vanishes and we show with numerical experiments that it is able to reproduce subtle properties of the Optimal Transport problem.

## 6.5. Phase retrieval for wavelet transforms

I. Waldspurger

[15]

This article describes an algorithm for solving a particular phase retrieval problem, with important applications in audio processing: the reconstruction of a function from the modulus of its wavelet transform. Previous algorithms for this problem were either unreliable in certain regimes, or too slow to be applied to largedimensional audio signals. Ours relies on a new reformulation of the phase retrieval problem, that involves the holomorphic extension of the wavelet transform. Numerical results, on audio and non-audio signals, show it allows precise reconstruction, and is stable to noise. Its complexity is linear in the size of the unknown signal, up to logarithmic factors. It can thus be applied to large signals.

# 6.6. Phase retrieval with random Gaussian sensing vectors by alternating projections

I. Waldspurger

[16]

We consider the phase retrieval problem that consists in reconstructing a vector from its phaseless scalar products with sensing vectors independently sampled from complex normal distributions. In the previous two years, several new non-convex algorithms have been introduced to solve it, and have been proven to succeed with high probability. In this work, we show that the same success guarantees hold true for the oldest and most well-known phase retrieval algorithm, namely alternating projections (Gerchberg-Saxton), provided that it is carefully initialized. We conjecture that this result is still true when no special initialization procedure is used, and present numerical experiments that support this conjecture.

## 6.7. Exponential decay of scattering coefficients

I. Waldspurger

[19]

The scattering transform is a deep representation, defined as a cascade of wavelet transforms followed by the application of a complex modulus. In her PhD, the author showed that, under some conditions on the wavelets, the norm of the scattering coefficients at a given layer only depends on the values of the signal outside a frequency band whose size is exponential in the depth of the layer. This article succintly describes this result, and generalizes it by removing one of the assumptions on the wavelets (namely the weak analyticity condition).

## 6.8. Generalized incompressible flows, multi-marginal transport and Sinkhorn algorithm

J-D. Benamou and G. Carlier and L. Nenna

[24]

Starting from Brenier's relaxed formulation of the incompressible Euler equation in terms of geodesics in the group of measurepreserving diffeomorphisms, we propose a numerical method based on Sinkhorn's algorithm for the entropic regularization of optimal transport. We also make a detailed comparison of this entropic regularization with the so-called Bredinger entropic interpolation problem. Numerical results in dimension one and two illustrate the feasibility of the method.

## 6.9. A Characterization of the Non-Degenerate Source Condition in Super-Resolution

V. Duval

[34]

This article deals with the Basis Pursuit (or LASSO) for measures for for the super-resolution problem, *i.e.* retrieving the fine details of a signal or an image. If the signal is made of M non-negative Dirac masses, under some assumptions on the measurement process, it is possible to exactly recover the signal from 2M observations, regardless of the minimum distance between the spikes. We study the stability to noise of such a reconstruction, and we propose a characterization of the *Non-Degenerate Source Condition* which is an almost necessary and sufficient for the stability of the support (the number and locations of the reconstructed spikes). The case of Laplace and Gaussian measurements are studied in detail.

## 6.10. A Low-Rank Approach to Off-The-Grid Sparse Deconvolution

P. Catala, V. Duval and G. Peyré

## [28].

We propose a new solver for the sparse spikes deconvolution problem over the space of Radon measures. A common approach to off-the-grid deconvolution considers semidefinite (SDP) relaxations of the total variation (the total mass of the absolute value of the measure) minimization problem. The direct resolution of this SDP is however intractable for large scale settings, since the problem size grows as  $f_c^{2d}$  where  $f_c$  is the cutoff frequency of the filter and d the ambient dimension. Our first contribution introduces a penalized formulation of this semidefinite lifting, which has low-rank solutions. Our second contribution is a conditional gradient optimization scheme with non-convex updates. This algorithm leverages both the low-rank and the convolutive structure of the problem, resulting in an  $O(f_c^d \log (f_c))$  complexity per iteration. Numerical simulations are promising and show that the algorithm converges in exactly r steps, r being the number of Diracs composing the solution.

## 6.11. Approximate Optimal Designs for Multivariate Polynomial Regression

*Y. De Castro* [110].

We introduce a new approach aiming at computing approximate optimal designs for multivariate polynomial regressions on compact (semi-algebraic) design spaces. We use the moment-sum-of-squares hierarchy of semidefinite programming problems to solve numerically the approximate optimal design problem. The geometry of the design is recovered via semidefinite programming duality theory. This article shows that the hierarchy converges to the approximate optimal design as the order of the hierarchy increases. Furthermore, we provide a dual certificate ensuring finite convergence of the hierarchy and showing that the approximate optimal design can be computed numerically with our method. As a byproduct, we revisit the equivalence theorem of the experimental design theory: it is linked to the Christoffel polynomial and it characterizes finite convergence of the moment-sum-of-square hierarchies.

## **NACHOS Project-Team**

## 6. New Results

## 6.1. Electromagnetic wave propagation

#### 6.1.1. 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 coupled 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. This is the object of the submitted paper [41]. At the same time, we pursue a study in collaboration with Serge Nicaise (Université de Valenciennes et du Hainaut-Cambresis) on the stability properties of this model both at the continuous and the discrete level.

### 6.1.2. Numerical modeling of metasurfaces

Participants: Loula Fezoui, Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Ronan Perrussel [Laplace laboratory, Toulouse].

Metamaterials are composed of periodic subwavelength metal/dielectric structures that resonantly couple to the electric and/or magnetic components of the incident electromagnetic fields, exhibiting properties that are not found in nature. Planar metamaterials with subwavelength thickness, or metasurfaces, consisting of a layer of dielectric or plasmonic nanostructures, can be readily fabricated using lithography and nanoprinting methods, and the ultrathin thickness in the wave propagation direction can greatly suppress the undesirable losses. Metasurfaces enable a spatially varying optical response, mold optical wavefronts into shapes that can be designed at will, and facilitate the integration of functional materials to accomplish active control and greatly enhanced nonlinear response. Designing metasurfaces is generally a challenging inverse problem. A recently introduced synthesis techniques is based on so-called General Sheet Transition Conditions (GSTC) that can be leveraged to define the components of general bianisotropic surface susceptibility tensors characterizing the metasurface. A GSTC-based design technique has several advantages: 1) it is exact; 2) it is general, transforming arbitrary incident waves into arbitrary reflected and transmitted waves, 3) it often admits closed-form solutions, 4) it provides deep insight into the physics of the transformations, 5) it allows multiple (at least up to 4) simultaneous and independent transformations. We study the numerical treatment of GSTC in the time-domain and frequency-domain regimes in the DG and HDG settings respectively.

#### 6.1.3. Corner effects in nanoplasmonics

**Participants:** Camille Carvalho [Applied Mathematics Department, University of California Merced, USA], 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.

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 that form a parametrized family of solutions. 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. This is the object of the submitted paper [37] (currently under a minor revision process).

## 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. This work has been presented in 2017 in one conference (see [32] and at the occasion of an invitation for a seminar (see section Invited talks).

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

**Participants:** Alexis Gobé, 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. The corresponding paper submitted at the end of 2016 is currently under revision (preprint available on HAL [14]). This work has also been presented in a conference in 2017, see [33]





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 [MIT, USA], Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.

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. As a preliminary step, we have investigated a fully explicit HDG method generalizing the classical upwind flux-based DG method for the system of time-domain Maxwell equations. We have study the stability of this new HDG method and in particular, the influence of the stabilization parameter on the CFL condition. We are now assessing the consitions under which we can obtain a superconverging HDG method.

#### 6.1.8. HDG methods for the frequency-domain Maxwell equations

Participants: 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 flexibility 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-conforming 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 frequency-domain plasmonics

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

In this collaboration with physicists at DTU Fotonik, we study HDG methods for solving the frequencydomain 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 the 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 have been implemented and numerically assessed for two-dimensional problems. Beside, we are also considering the three-dimensional case

#### 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, Weslley Da Silva Pereira [LNCC, Petropolis, Brazil], 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. Porting 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.



Figure 5. DEEP-ER hardware architecture sketch.

## 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 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.

## 6.4. Applications

#### 6.4.1. Light transmission in subwavelength gratings

**Participants:** Leandro Andrade Couto Fonseca, Hugo Enrique Hernandez Figueroa [Universidade Estadual de Campinas, Sao Paulo, Brazil], Laurent Labonté [Information Quantique avec la Lumière et la Matière (QILM) team, INPHYNI, Université Nice Sophia Antipolis], Stéphane Lanteri, Jonathan Viquerat.

Silicon photonics has great potential to bringing together two technological areas that have transformed the last century, electronics and photonics. Silicon waveguides are important components for tailoring photonic functions on silicon. They have been studied extensively over the pas two decades. There are a number of waveguide geometries that have been developed in silicon. The most common are strip waveguides, rib waveguides and slot waveguides. The Bragg grating is a fundamental component in various optical devices and has applications in areas as diverse communications, laser and sensors. In the simplest configuration, a Bragg grating is a structure with periodic modulation of the effective refractive index. This modulation is commonly achieved by varying the refractive index (e.g. alternating material) or the physical dimensions of the waveguide. At each boundary, a reflection of the travelling light occurs, and the relative phase of the reflected signal is determined by the grating period and the wavelength. The repeated modulation of the refractive index results in multiple and distributed reflections. The reflected signals only interfere constructively in



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.

a narrow band around one particular wavelength, namely the Bragg wavelength. Within this range, light is strongly reflected. At other wavelengths, the multiple reflections interfere destructively and cancel each other out, and as a result, light is transmitted through the grating. This is the functional principle of the concept SubWavelength Gratings (SWG). In the context of the OPENING (On-chiP wirEless quantum state eNgineerING) project of the UCA JEDI Excellence Inititiave, we collaborate with the QILM team of the INPHYNI laboratory, on the numerical modeling of light propagation in SWG waveguides, suing a high order DGTD solver from the DIOGENeS software suite. Two situations are considered: (1) in a first step, an ideal configuration corresponding to a virtual design will be simulated; (2) in a second step, several deformed configurations, which are more in line with actual designs (i .e. from lithography), are studied with the goal of identifying the main sources of performance degradation from the transmission point of view.

#### 6.4.2. Light diffusion in nanostructured optical fibers

**Participants:** Wilfried Blanc [Optical Fibers team, INPHYNI, Université Nice Sophia Antipolis], Stéphane Lanteri, 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 (INPHYNI) 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.

#### 6.4.3. Gap-plasmon confinement with gold nanocubes

**Participants:** Stéphane Lanteri, Antoine Moreau [Institut Pascal, Université Blaise Pascal], Armel Pitelet [Institut Pascal, Université Blaise Pascal], Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.





Figure 7. Partial view of a SWG wavewguide tetrahedral mesh (top left); reflection and transmission coefficients (bootom).1



Figure 8. Unstructured tetrahdral mesh of a nanostructured optical fiber core.

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. 9). The behavior of single nanocubes on metallic plates has been simulated, for lateral sizes c ranging from 50 to 80 nm, and spacer thicknesses  $\delta$  from 3 to 22 nm. The absorption efficiency in the cube  $Q_{\text{cube}}$  at the resonance frequency is retrieved from the results of each computation (see Fig. 10).





Figure 9. 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.

#### 6.4.4. Light-trapping in nanostructured solar cells

**Participants:** Urs Aeberhard [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Karsten Bittkau [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Alexis Gobé, Stéphane Lanteri.

This work is undertaken in the context of the EoCoE Center of Excellence in collaboration with researchers from IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, Germany. The objective is to design a scalable high order DGTD solver for the simulation of light trapping in a multi-layer solar cell with surface texture. For that purpose, we rely on the DIOGENeS software suite from which we extract a high order DGTD solver for the problem under consideration, taking into account its specificities (in particular, with regards to material models and boundary conditions). We also need to specify and develop a dedicated preprocessing tool for building topography conforming geometrical models. Simulations are performed on the Occigen PRACE system at CINES.


 $c = 70 \text{ nm}, \delta = 12 \text{ nm}$   $c = 60 \text{ nm}, \delta = 18 \text{ nm}$ Figure 10. 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.



Figure 11. Simulation of light trapping in a multi-layer solar cell with surface texture using a high order DGTD fullwave solver and topography conforming geometrical models.

## **NANO-D Project-Team**

## **5. New Results**

#### 5.1. Incremental methods for long range interactions

Participants: Semeho Edorh, Stephane Redon.

Adaptively Restrained Molecular Dynamics (**ARMD**) 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 **ARMD** to electrostatic simulations. Therefore, we developed a fast method dedicated to the computation of the electrostatic potential in adaptively restrained systems. The proposed algorithm is derived from a multigrid-based alternative to the popular particle mesh methods. Our algorithm ,labeled as Incremental Mesh Continuum Method (IMCM),was implemented inside LAMMPS, a popular molecular dynamics simulation package. During ARMD simulations, IMCM scales with the number of active particles.

The performance of the new algorithm was accessed on various molecular systems. 1 showed that IMCM is able to outperform the well-established Particle Particle Particle Mesh (P3M) for adaptively restrained simulations. For an aqueous solution of sodium chloride, water molecules can be adaptively restrained. On this system, ARMD was able to reproduce static properties of sodium chloride (2). When a functionalized nanopore is placed at the center of the system, ARMD and IMCM were able to reproduce the ion selectivity property (3). For this benchmark, this positively charged nanopore acts like a sieve that blocks the flux of Sodium atoms, while promoting the crossing of Chlorine particles(4).

## 5.2. Adaptive Algorithms for Orbital-Free Density Functional Theory

Participants: Francois Rousse, Stephane Redon.

Our Orbital-Free Density Functional Theory (OF-DFT) program has been enriched and improved. Its accuracy has been demonstrated just like in he work of [79] : by comparison with the PROFESS software [47] of energies and relaxed geometries of several aluminium clusters. An incremental version has been developed and tested: it can be tuned smoothly from fast and approximative to slow and precise. We have shown that for cases where few particles positions have changed, like in an adaptively restrained dynamical [23], the update of electronic density is faster with the adaptive version.

A SAMSON App computing electronic energies through Orbital-Free DFT has been released for SAMSON 0.6.0. It is a light version, with only one optimization algorithm and no adaptive version. The parallel implementation is available for most operating systems. Another SAMSON App is being developed to generate the input files of PROFESS, our reference software for OF-DFT.

#### 5.3. As-Rigid-As-Possible molecular interpolation paths

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

We proposed a new method to generate interpolation paths between two given molecular conformations [11]. It relies on the As-Rigid-As- Possible (ARAP) paradigm used in Computer Graphics to manipulate complex meshes while preserving their essential structural characteristics. Experiments conducted on a large set of benchmarks show how such a strategy can efficiently compute relevant interpolation paths with large conformational rearrangements.



Figure 1. Performance depending on the percentage of active particles for different number of processes. Performance of LAMMPS P3M is shown as a reference (dotted lines, pentagram marker) — it does not depend on the percentage of active particles. In all cases electrostatics were computed at similar accuracy ( $\sim 10^{-5}$ ).



Figure 2. Ion-water pair distribution functions using armd with the NaCl/ $\epsilon$  force field at 298 K the rigid water model SPC/ $\epsilon$  and an ionic concentration of 10.0 molal. Different restraining parameters ( $\varepsilon^r$ ,  $\varepsilon^f$ ) were tested on water molecules. Na and Cl are always active. Black line corresponds to a standard molecular dynamics simulation of the system.



Figure 3. Number density of chlorine (red dotted line) and sodium (blue dashed line) ions along z-axis using standard ARMD (Left) and MD (Right). Both methods show the ion selectivity of the nanopore which is located at z = 0.

## 5.4. ART-RRT: As-Rigid-As-Possible Exploration of Ligand Unbinding Pathways

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

We proposed a method to efficiently generate approximate ligand unbinding pathways (to appear in the Journal of Computational Chemistry). It combines an efficient tree-based exploration method with a morphing technique from Computer Graphics for dimensionality reduction. This method is computationally cheap and, unlike many existing approaches, does not require a reaction coordinate to guide the search. It can be used for finding pathways with known or unknown directions beforehand. The approach is evaluated on several benchmarks and the obtained solutions are compared with the results from other state-of-the-art approaches. We show that the method is time-efficient and produces pathways in good agreement with other state-of-the-art solutions. These paths can serve as first approximations that can be used, analyzed or improved with more specialized methods.

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

Participants: Jaillet Leonard, Svetlana Artemova, Stephane Redon.

IM-UFF, the extension of UFF to interactive modeling was completed. It led to an analysis demonstrating that IM-UFF allows to obtain statistical measures that are normally only accessible to reactive force fields (cf. Figure 7). It resulted in the paper "IM-UFF: extending the Universal Force Field for interactive molecular modeling" published at the Journal of Molecular Graphics and Modelling [7]. IM-UFF will be proposed as a module available to all public in the 0.7.0 version of SAMSON that will be released soon.

#### **5.6. Exploring Chemical Reaction Paths**

Participant: Jaillet Leonard.



Figure 4. Nonuniform distributions of number density of chlorine (Top) and sodium (Bottom) ions driven by an external electric field (black arrow) E = 1 V/A using standard MD (Left) and ARMD (Right). The gray rectangles at z = 0 mark the graphene sheet. Both ions form concentration polarization layers.



Figure 5. Motion of Adenylate Kinase from "open" to "close" state generated with the ARAP method.



Figure 6. Paths (in colored sticks) obtained by ART-RRT for the unbinding of retinoic acid hormone from its receptor. The protein is represented by ribbons and the ligand by orange balls. Two different views are shown for clarity. The left picture shows pathways I in red, II in blue, III in green and Other in black. The right picture shows pathways IV in yellow, V in purple and VI in cyan. These main pathways are also reported by other studies by the SMD and RAMD methods for nuclear hormone receptors.



Figure 7. The interaction between 10 methane molecules restrained in a fixed volume is simulated through Monte Carlo simulation (left). The radial distribution functions (RDF) obtained with Brenner (blue curves) are qualitatively the same as those obtained with IM-UFF (red curves), in case of a 500 K temperature setup (top) as well as a 7000 K temperature setup (bottom). It means that, it might be possible to use IM-UFF to obtain statistical measures that are normally only accessible to reactive force fields.

#### 5.6.1. Context

In the past, we have developed a methodology to explore chemical reaction paths based on stochastic trees. One difficulty was the assessment of the quality of the paths found, and the comparison with existing state of the art methods.

To address these limitations, we have developed several new modules in SAMSON that propose state of the art methods and helpful tools to find and manipulate the paths and the important states of the considered systems. One can classify these modules into three categories: interpolation methods, minima and saddle point search methods and supporting tools. More details regarding these modules are provided below.

#### 5.6.2. Interpolation methods

We have implemented the artificial force induced reaction (AFIR) method [59], that helps to find a transition path from a given initial state made of two compounds A and B, towards a goal compound X. In the futur, we would like to combine AFIR with our exploration methods.

The Linear Synchronous Transit (LST) and the Quadratic Synchronous Transit (QST) methods [42] have also been integrated in SAMSON. These methods generate paths such that each atom-pair distance in an intermediate structure is the interpolated value between those in the initial and target structures. The QST variant differs of the LST one from that the interpolated path also passes through a third intermediate point. Moreover, we have implemented the MINIMAX method as in [50] that alternates phases of minimization and QST interpolation to search for a transition path. These three methods appear to show a better behavior than a simple linear interpolation approach. In the future, we are also planning to combine them with our exploration methods.

#### 5.6.3. Search for minima and saddle points

We have developed a SAMSON module to describe the energy basins associated to the various conformations of a given set. For this, conformations are first minimized and then clustered. This tool is also convenient when analyzing conformations along a given path to search for the states the closest to the saddle points.

In collaboration with the post doc Clément Betone, we have implemented two modules. First, the Dimer method as proposed in [45]. This method allows to find from a given point the closest saddle points in high dimensional potential surfaces, using only first derivatives. Some works remains to be done to solve the sensibility problem related to the initial orientation of the dimmer. Second, the freezing string method as proposed in [24]. This method searches efficiently for a saddle point between two given end states through a combination of interpolatoin and optimization.

To assess the various methods and obtain a visual feedback of their behavior, we have developed several 2D force fields where the energetical landscape can easily be apprehended. Such an example of landscape is illustrated in Figure 8.



Figure 8. Example of 2D force field used to test the various methods performing force field searches. One can see at the bottom right, the current state represented by a red cross and at a local minimum

#### 5.6.4. Supporting tools

We have proposed in SAMSON a set of tools to manipulate and perform some measures associated to set of conformations, that could potentially represent molecular paths.

A first tool was proposed to perform given measures for a given set of conformations, such as bond lengths, angle bends, or torsion angles. A second tool allows to align various conformations onto a reference on. Finally, another tool allows to compute the RMSD distance between pairs of conformations.

## 5.7. Combination of force fields

We have proposed in SAMSON several modules related to force fields, that can be used as soft constraints applied to a system. We have proposed a force field that sums up the contributions of two given force fields for a given system. Another force field was developed based on three force fields, where the first one concerns one part of the system, the second one an another part and the last one the interaction between these two parts. We have also added elementary force fields for the standard interactions that may be represented classical force fields: bond springs, angle bend springs, torsion springs, Steric clash and Van der Waals interactions.

#### 5.8. Simulating nanomaterials

We have initiated an informal collaboration with Cyril Guedj, a permanent researcher of the Leti at CEA. This researcher is an expert in nanomaterials and the goal is to develop in SAMSON tools to manipulate, simulate and measure these nanomaterials. We focused in particular in crystals that appears in many new materials such as semiconductors.

So far, we have developed three versions of Keating for simulating crystals: an harmonic Keating force field for elements of type IV based on [55], an harmonic Keating force field extended to elements of type III and V based on [30] and a non-harmonic Keating force field based on [74]. An example of crystal simulated with Keating force field in SAMSON is shown in Figure 9 Currently, we are in a phase of validation of these force fields. Cyril Guedj as experts in nanomaterials is focusing on the calibration of the force field parameters and the comparison with state of the art results. In the future, we plan to extend the functionality of these force fields to address more complex scenarii.

In parallel, we have developed a set of tools to manipulate and measure these crystal: a module to rescale them, one to simplify their visualization, one to measure a set of characteristics, and finally, one to simulate constraints applied to some part of the system.



Figure 9. Example of crystal simulated in SAMSON, using one variant of the Keating force field.

#### 5.9. Parallel algorithms for adaptive molecular dynamics simulations

Participants: Dmitriy Marin, Stephane Redon.

We worked on the development and improvement of a parallel implementation of the Adaptively Restrained Molecular Dynamics (ARMD) method in the LAMMPS molecular dynamics simulator. The parallelization was done in application to multi-core CPU and hybrid CPU/GPU systems thanks to the Kokkos package provided by LAMMPS. The ARMD can be used for decreasing computational complexity by restraining degrees of freedom for some particles in the simulated system [23], therefore allowing to gain speed-up by either decreasing precision or focusing on select subsystems. The developed parallel implementation allows us to run LAMMPS with an ARMD integrator on central processing units (CPU), graphics processing units (GPU), and many integrated core architecture (MIC). We developed a new algorithm for processing particles that switches their state from a restrained state to a full-dynamics state and vice versa. The new algorithm is modified for efficient usage of GPU and many-core CPUs (computations are performed on a computational device, communications between host and device are decreased). The results on performance and speed-up for ARMD in comparison with the non-modified LAMMPS for a standard Lennard–Jones liquid benchmark are shown in Figures 10 and 11. We showed that starting from some number of atoms in the system and from some percentage of restrained atoms, ARMD provides better performance over classical MD. The results are published in [14].

# 5.10. Development of Convex-PL, a scoring function for protein-ligand interactions

Participants: Sergei Grudinin, Maria Kadukova.



*Figure 10. Performance for a system with ARMD parameters:*  $\varepsilon^r = 4.5$ ,  $\varepsilon^f = 6.5$ 



Figure 11. Speed-up for a system with 1 372 000 atoms



Figure 12.

We have continued developing Convex-PL, which is a knowledge-based scoring function for protein-ligand interactions. It is based on the assumption that protein-ligand interactions linearly depend on radial distributions of pairs of atoms of various types. The corresponding coefficients are deduced with a convex optimization problem from the structural data. We augmented Convex-PL with a term standing for steric clashes, ran a leave-one-out cross-validation procedure, and additionally validated it on the D3R Grand Challenge 2 usersubmitted poses. The corresponding paper [8] was accepted to the Journal of Computer-Aided Molecular Design. We have also presented Convex-PL at two scientific conferences [53], [52].

# 5.11. Participation in the D3R Grand Challenge 2 with the Convex-PL scoring function

Participants: Sergei Grudinin, Maria Kadukova.



Figure 13. Structural heterogeneity of the target FXR proteins.

We have participated in the pose prediction stage of the D3R Grand Challenge 2 using Convex-PL to re-score the ligand poses obtained with Autodock Vina. The target protein of this challenge was a farnesoid X receptor (FXR). After the correct co-crystal poses were released, we carefully repeated the experiments and compared them with several other docking protocols. For these protocols we have used a modified version of Autodock Vina with Convex-PL as a built-in scoring function used in sampling. The protocols we have tried include comparison of docking to various co-crystal and mutated co-crystal FXR structures, as well as docking to the correct protein structures to evaluate the influence of receptor flexibility and docking of ligand structures generated with two different algorithms, as well as the co-crystal ones. This study was published in the Journal of Computer-Aided Molecular Design. [9]

## 5.12. Development of a Normal Modes Analysis SAMSON Element

Participants: Yassine Naimi, Alexandre Hoffmann, Sergei Grudinin.

We developed a SAMSON Element based on the method proposed by Alexandre Hoffman and Sergei Grudinin on Linux and Mac operating systems. This SAMSON Element was implemented in two versions, a Lite version and an Advanced version.



Figure 14. Normal Modes Analysis element Lite version.

The first one (14) computes the nonlinear normal modes of a molecular system (protein, RNA, DNA) very quickly using the NOLB algorithm developed by Alexandre Hoffmann and Sergei Grudinin (J. Chem. Theory Comput., 2017, 13 (5), pp 2123-2134, DOI: 10.1021 / acs.jctc.7b00197.). The user indicates the desired number of modes, the interactions cutoff distance and the potential function. For now, the elastic network model potential is the one that is available but more potential functions, like the Gaussian network model, will be added in the future. In the output, each mode is represented by a slider. The user can visualize the motion of each mode independently by moving its corresponding slider manually or by checking its checkbox and then pressing on the play button. Also, the user can visualize the motion of a combination of modes selecting them before playing the motion.

The transformations used in this motion can be set to linear or nonlinear and the amplitude of the motion can be increased/decreased by changing the scaling factor. During this motion, the user can activate a real time minimization using one of the provided algorithms (steepest descent, conjugated gradient or LBGF) and defined values of minimization steps and minimization tolerance. Finally, the user can either save/export a given conformation of the structure or the entire displayed trajectory by going into the "Save Frames" tabulation of the SAMSON element.



Figure 15. Normal Modes Analysis element Advanced version (A)

The second one (15) is an advanced version of the Nonlinear Normal Modes Analysis module. It computes the nonlinear normal modes of a molecular system (protein, RNA, DNA) in the same time given that it uses the same algorithm developed by Alexandre Hoffmann and Sergei Grudinin (J. Chem. Theory Comput., 2017, 13 (5), pp 2123-2134, DOI: 10.1021 / acs.jctc.7b00197.). It has the same functionalities than the Lite version of the Normal Modes Analysis element. In addition, the element has an additional tabulation called "Structure Definition" (16). In this section, users can define a pocket and ask for a combination of modes that contribute the most to the opening and closing of this pocket. Also, in the near future, another functionality will be added in the "Structure Definition" tabulation called "reference structure definition". Using this functionality, users can define the conformation of structure as a reference and the element will provide a combination of modes that will lead this structure to present this conformation.

#### 5.13. Development of a Hex SAMSON Element

Participants: Yassine Naimi, Sergei Grudinin.

We developed a SAMSON Element to wrap Hex (17), an interactive protein docking software, written by Dave Ritchie (LORIA/Inria Nancy). With this element, users can define receptor/ligand structures displayed



Figure 16. Normal Modes Analysis element Advanced version (B)



Figure 17. Hex element.

in the SAMSON viewport or import their PDB files. All the options available on the Hex software have been implemented in this SAMSON element.



Figure 18. Hex results.

Then, by clicking on the Run button, docking solutions will be computed and clustered in a table (18) using the Hex algorithm. Users can show the resulted docking solutions by clicking on the play button, or the solution line in the table or the next/previous buttons.

## 5.14. Development of RDKit Smiles Manager SAMSON Elements

#### Participant: Yassine Naimi.

We integrated RDKit, an open-source collection of cheminformatics and machine-learning software written in C++ and Python, in SAMSON. One of RDKit's features is the conversion of molecules from their SMILES code to a 2D and 3D structures. Therefore, it is now possible to use these features in the SAMSON platform. SMILES code files (.smi) or text files (.txt) containing several SMILES codes can be read using the import button (19).

Users can manage the imported data with several manners (modify the SMILES code, add manually a new SMILES code, assign names to the molecules...). Also, 2D depictions of the SMILES code are generated on the fly (20). When a SMILES code is invalid an error image is automatically generated. By right-clicking on these images, users can open or generate the 3D structure in SAMSON or save the image as png or svg. The main feature of this element is to generate 3D structures from imported/written SMILES codes. After selecting the molecules, users can click on the Generate 3D structures button. Few seconds later, the 3D structures of the molecules (presenting a valid SMILES code) are added to the SAMSON document view. Finally, RDKit provides a feature to filter the selected molecules using a substructure pattern (SMILES or SMARTS). By default in RDKit, information about stereochemistry is not used in substructure searches but this can be changed by using the chirality. For information, the name of the molecules that did not include the given pattern are displayed in a pop-up.

## 5.15. Symmetry mate generator for SAMSON

Participants: Guillaume Pagès, Sergei Grudinin.



Figure 19. RDkit Smiles Manager element.

🐵 RDKit-SMILES Manager		■ 🔒 ? 🗙
Smiles Code		
Import From File: C:/Users/naimi/Desktop/smileFile.smi		Import
Select All Cleartable		
Name	Code	2D Conformation
1 C1cccn(=O)c1	c1cccn(=O)c1	
2 🗹 C==	C==	Syntax error in SMILES string
Substructure Filtering  Substructure Filtering  Generate 3D structures		

Figure 20. RDkit Smiles Manager element.



Figure 21. The Symmetry Mate element.

Many biological systems are composed of several identical units structurally organized in a symmetric manner. To observe the atomistic contacts in a system, one needs to replicate the asymmetric unit and apply specific rigid-body operations to it. We developed a SAMSON element that is able to read these operations from a file, and which provides a way to replicate the subunits in a user-friendly fashion.

## 5.16. Development of a symmetry detection software AnAnaS

Participants: Guillaume Pagès, Sergei Grudinin.

Macromolecules are generally not rigid bodies at physiological temperature and they adopt different conformational states. Thus, if one considers a macromolecular assembly made of N subunits, do we expect that all the units will be structurally identical to each other? Most probably not, since at any given moment of time, each unit may be sampling a different conformational state. For example, there are plenty of X-ray structures of homo-dimers, where the individual monomers are not structurally identical.

In order to quantitatively assess these differences, we developed a method for Analytical Analysis of Symmetries (AnAnaS) in protein complexes. The method is extremely fast, robust and accurate. Two manuscripts describing the method are currently submitted for publication. This method is available on the website of the team (https://team.inria.fr/nano-d/software/ananas/).

#### 5.17. Integration of AnAnaS to SAMSON

Participants: Guillaume Pagès, Sergei Grudinin.

We created a SAMSON element to make the symmetry detection and symmetry axes' visualization as easy and intuitive as possible.

## 5.18. Deep Learning for Symmetry detection

Participants: Guillaume Pagès, Sergei Grudinin.

We are working on a fully-structural method for detecting symmetries in molecular structures. This will allow us to detect tandem repeats, or even symmetry in density maps. We created a method based on neural network and deep learning, inspired by the advances in computer vision in the past decade. According to our first tests on simulated examples, our method is able to detect the order of a cyclic symmetry (which can be 1 for asymmetric structure) with a 92% accuracy, and guesses the direction of the axis of symmetry with an average error of  $3^{\circ}$ . We are still working on improving it and doing tests on more realistic examples.



Figure 22. System with an octahedral symmetry, with the axes displayed in SAMSON.

## 5.19. Pepsi-SAXS calculator of small-angle X-ray scattering profiles

Participants: Sergei Grudinin, Maria Garkavenko.

We have continued the development of a new method called Pepsi-SAXS that calculates small angle X-ray scattering profiles from atomistic models [2]. The method is based on the multipole expansion scheme and is significantly faster with a comparable precision than other methods.

Our method has been highlighted in a recent SAXS-related review [49] and was one of the best performers in the recent CASP12 data-assisted protein structure prediction experiment [81].

Pepsi-SAXS is available at http://team.inria.fr/nano-d/software/pepsi-saxs. A SAMSON module will be made available at https://www.samson-connect.net.

## **5.20. NOLB nonlinear normal modes**

Participants: Alexandre Hoffmann, Sergei Grudinin.

We developed a new conceptually simple and computationally efficient method for nonlinear normal mode analysis called NOLB [4]. This is a logical evolution of the RTB-subspace method developed by Y.-H. Sanejouand and colleagues [38], [80]. We demonstrated how to physically interpret the eigenvalues computed in the RTB basis in terms of angular and linear velocities applied to the rigid blocks and how to construct a nonlinear extrapolation of motion out of these velocities. The key observation of our method is that the angular velocity of a rigid block can be interpreted as the result of an implicit force, such that the motion of the rigid block can be considered as a pure rotation about a certain center.

Overall, our method produces better structures compared to the standard approach, especially at large deformation amplitudes, as we demonstrate by visual inspection, energy and topology analyses, and also by the MolProbity service validation. Also, our method is scalable and can be applied to very large molecular systems, such as ribosomes.

Standalone executables of the NOLB normal mode analysis method are available at https://team.inria.fr/nanod/software/nolb-normal-modes/. A graphical user interface created for the SAMSON software platform will be made available at https://www.samson-connect.net.

## 5.21. Applications of the NOLB NMA method to structural biology

Participant: Sergei Grudinin.



Figure 23.



Figure 24.

#### Participants: Sergei Grudinin

Using the created nonlinear normal mode analysis NMA tool, we have successfully predicted structural transitions in several protein complexes, whose structures were solved by our collaborators [6], [3].

## 5.22. Off-grid fitting method

Participants: Alexandre Hoffmann, Sergei Grudinin.





We developed a novel Fast Fourier Transform (FFT)-based exhaustive search method extended to off-grid translational and rotational degrees of freedom [5]. The method combines the advantages of the FFT-based exhaustive search, which samples all the conformations of a system under study on a grid, with a local optimization technique that guarantees to find the nearest optimal off-grid conformation. The method is demonstrated on a fitting problem and can be readily applied to a docking problem.

The algorithm first samples a scoring function on a six-dimensional grid of size  $N^6$  using the FFT. This operation has the asymptotic complexity of  $O(N^6 \log N)$ . Then, the method performs the off-grid search using a local quadratic approximation of the cost function and the trust region optimization algorithm. The computation of the quadratic approximation is also accelerated by FFT at the same additional asymptotic cost of  $O(N^6 \log N)$ . We demonstrate our method on fitting atomic protein models into several simulated and experimental maps from cryo-electron microscopy. The method is available at https://team.inria.fr/nano-d/software/offgridfit.

## 5.23. RapidRMSD library

Participants: Emilie Neveu, Petr Popov, Sergei Grudinin.

The root mean square deviation (RMSD) is one of the most used similarity criteria in structural biology and bioinformatics. Standard computation of the RMSD has a linear complexity with respect to the number of atoms in a molecule, making RMSD calculations time-consuming for the large-scale modeling applications, such as assessment of molecular docking predictions or clustering of spatially proximate molecular conformations. Previously we introduced the *RigidRMSD* algorithm to compute the RMSD corresponding to the



Figure 26.

rigid-body motion of a molecule [62]. Recently, we went beyond the limits of the rigid-body approximation by taking into account conformational flexibility of the molecule. We model the flexibility with a reduced set of collective motions computed with e.g. normal modes or principal component analysis.

The initialization of our algorithm is linear in the number of atoms and all the subsequent evaluations of RMSD values between flexible molecular conformations depend only on the number of collective motions that are selected to model the flexibility. Therefore, our algorithm is much faster compared to the standard RMSD computation for large-scale modeling applications. The method can be applied e.g. to cluster flexible docking or to generate pseudo-random constant-RMSD structural molecular ensembles.

The algorithm is written in C++ as the open-source *RapidRMSD* library governed by the BSD-compatible license, which is available at http://team.inria.fr/nano-d/software/RapidRMSD/. The constant-RMSD structural ensemble application is available at http://team.inria.fr/nano-d/software/nolb-normal-modes/.

## 5.24. SBROD protein quality assessment method

Participants: Mikhail Karasikov, Sergei Grudinin.

Protein quality assessment (QA) is a crucial element of protein structure prediction, a fundamental but yet open problem in structural bioinformatics. QA aims at ranking predicted protein models from a set of proposed candidates. Although consensus-model QA methods often outperform single-model QA methods, their performance substantially depends on the pool of available candidates. This makes single-model QA methods a particularly important research target since these usually assist in the sampling of candidates.

We developed a novel single-model QA method called SBROD. The SBROD (Smooth Backbone-Reliant Orientation-Dependent) method uses only the conformation of the protein backbone, and hence it can be applied to scoring the coarse-grained protein models. The proposed method deduces the scoring function from a training set of protein models. This function is composed of four terms related to different structural features, residue-residue orientations, contacts between the backbone atoms, hydrogen bonding, and solvent-solvate interactions. The SBROD scoring function is smooth with respect to atomic coordinates and thus is applicable to continuous gradient-based optimization of protein conformations. Furthermore, it can also be used for coarse-grained protein modeling and computational protein design. Computational experiments conducted on diverse datasets (Stage1 and Stage2 from CASP11, and MOULDER) proved SBROD to achieve the state-of-the-art performance among single-model QA methods including meta algorithms.

The standalone application implemented in C++ and Python is freely available at https://team.inria.fr/nanod/software/SBROD and supported on Linux, MacOS, and Windows.



Figure 27.

## 5.25. Symmetry detection methods

Participants: Etienne Bamas, Sergei Grudinin.

We have developed a novel framework for the computational detection of point-group symmetries in electron density maps. The method is based on the symmetry-based reduced representation of the density using polynomial expansions.

#### 5.26. SAXS-assisted protein docking

Participants: Gaurav Dhar, Sergei Grudinin.

We have developed an extension of the Pepsi-SAXS method [2] applicable to rescoring of rigid-body proteinprotein docking predictions.

## 5.27. Methods for the estimation of collective motions

Participants: Robin Gullo, Sergei Grudinin.

We have studied novel ways to predict structural conformational transitions in macromolecules.

## 5.28. Smoothed-force energy optimization

Participants: Clement Beitone, Stephane Redon.

Many approaches have been developed during the last decades to improve the speed of convergence of optimization methods used to find minima of potential energy surfaces. We proposed to spatially and temporally smooth the force vector given by the force field. Our approach alters the deformation of the structure being minimized and makes it behave as if it was locally more rigid. We apply this filtering method to two well-known optimization methods, steepest descent and FIRE, and evaluate its efficiency on several benchmarks, including nanomaterials and biomolecules. We demonstrated that the smoothed force variants may significantly speed up energy minimization.

## 5.29. Adaptively Restrained Molecular Dynamics in LAMMPS

Participants: Krishna Kant Singh, Stephane Redon.

Adaptively Restrained Molecular Dynamics (ARMD) is a recently introduced particles simulation method that switches positional degrees of freedom on and off during simulation in order to speed up calculations. In the NVE ensemble, ARMD allows users to trade between precision and speed while, in the NVT ensemble, it makes it possible to compute statistical averages faster. Despite the conceptual simplicity of the approach, however, integrating it in existing molecular dynamics packages is non-trivial, in particular since implemented potentials should a priori be rewritten to take advantage of frozen particles and achieve a speed-up. We proposed novel algorithms for integrating ARMD in LAMMPS, a popular multipurpose molecular simulation package [12]. In particular, we demonstrated how to enable ARMD in LAMMPS without having to re-implement all available force fields. The proposed algorithms were assessed on four different benchmarks, and showed how they allowed us to speed up simulations up to one order of magnitude.

## 5.30. Single-pass Incremental Force Updates for Adaptively Restrained Molecular Dynamics

Participants: Krishna Kant Singh, Stephane Redon.

We proposed new, single-pass incremental force updates algorithms to efficiently simulate a system using ARMD [13]. We assessed different algorithms for speedup measurements and implemented them in the LAMMPS MD package. We validated the single-pass incremental force update algorithm on four different benchmarks using diverse pair potentials. The proposed algorithm allows us to perform simulation of a system faster than traditional MD in both NVE and NVT ensembles. Moreover, ARMD using the new single-pass algorithm speeds up the convergence of observables in wall-clock time.

## 5.31. Auto update process for SAMSON & SAMSON-SDK

Participant: Jocelyn Gate.

Since SAMSON 0.6.0, instead of manually installing the latest SAMSON updates, the existing SAMSON can keep itself up-to-date automatically. If an internet connection is established and as soon as we add a new version of SAMSON on SAMSON Connect, all users that launch SAMSON will be notified that a new version is available. The previous version will remain running until SAMSON is closed, but the updated version will be launched automatically the next time you start SAMSON. It is a one click process.

#### 5.31.1. The SAMSON auto update

When a new SAMSON is available users have a notification and a summary if all elements they use are still available in the updated version.

#### 5.31.2. The SAMSON-SDK auto update

When a new SAMSON-SDK is available users have notification and they can install it in one click when SAMSON starts.

## **5.32. SAMSON Elements policies**

Participants: Jocelyn Gate, Stephane Redon.

Some developers of SAMSON wanted to restrain access to their developed SAMSON Elements, hence we defined four different access policies:

- Private : only the developer and the collaborators can see and use the corresponding published element
- Public : everyone can see and use the corresponding published element
- Hidden : only users that get the corresponding hidden link can see and use the corresponding published element
- Shared : only the users that have been added to the list of shared users can see and use the corresponding published element



Figure 28. The update notification



Figure 29. The available element summary



Figure 30. The update progress



Figure 31. The policy configuration

## 5.33. Improvements to our software development pipeline

Participant: Jocelyn Gate.

In order to fully automate the deployment process we increased the number of jenkins features.

- SAMSON Element packaging and deployment for every NANO-D users to samson-connect.
- SAMSON & SAMSON-SDK documentation build.
- SAMSON & SAMSON-SDK documentation upload via FTP to the new documentation website. (https://documentation.samson-connect.net/)

## 5.34. SAMSON Connect Forum

Participants: Jocelyn Gate, Stephane Redon.

To help the community to use SAMSON and develop elements with the SAMSON SDK, we setup a forum thanks to Jean-Francois Scariot from Inria (https://forum.samson-connect.net/). Despite the fact that the samson-connect.net and forum.samson-connect.net websites are separate, the login functionality is shared, since the user logs in samson-connect.net to access the forum.

## **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 wavepropagation 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.

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. We have also proved the convergence of the discrete method with respect to the size of truncation of the Fourier integrals, and with respect to the mesh size. This is the object of a paper that has been submitted.

In parallel, the main ingredient for the numerical method in 3D has been developed. It is the modal/Fourier representation of the elastic field in a semi-infinite plate, as a function of the trace of the displacement and of the normal stress. This has been done in the isotropic case.

#### 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, Clément Beneteau.

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.

## 7.5. Spectral theory and modal approaches for waveguides

#### 7.5.1. 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.

#### 7.5.2. 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 and Vincent Pagneux from Laboratoire d'Acoustique de l'Université du Maine. 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 are used for the two different definitions of invisibility, leading to non-selfadjoint eigenvalue problems.

More precisely, for the case of no-reflection, we define a new complex spectrum which contains as real eigenvalues the frequencies where perfect transmission occurs and the frequencies corresponding to trapped modes. In addition, we also obtain complex eigenfrequencies which can be exploited to predict frequency ranges of good transmission. Our approach relies on a simple but powerful idea, which consists in using PMLs in an original manner: while in usual PMLs the same stretching parameter is used in the inlet and the outlet, here we take them as two complex conjugated parameters. As a result, they select ingoing waves in the inlet and outgoing waves in the outlet, which is exactly what arises when the transmission is perfect. This simple idea works very well, and provides useful information on the transmission qualities of the system, much faster than any traditional approach.

#### 7.5.3. 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 Dirichletto-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 stratified, 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. 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 (in the monomode regime) 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 low frequency and small perturbations. During the last year, we have shown that the previous idea can be combined with a continuation method, in order to get larger invisible perturbations at higher frequency.

## 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 Project-Team**

## 6. New Results

#### 6.1. Variational approach for multiphase flows

In [66], 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 [20] is then twofold. First, it extends the variational interpretation of [66] 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  $\dot{a} \, la$  Jordan, Kinderlehrer, and Otto [86] is shown in [20], providing by the way a new existence result for multiphase flows in porous media. The result relies on advances tools related to optimal transportation [94], [93].

Based on the previous work, Clément Cancès, Daniel Matthes, and Flore Nabet derived in [46] a model of degenerate Cahn-Hilliard type for the phase segregation in incompressible multiphase flows. The model is obtained as the Wasserstein gradient flow of a Ginzburg-Landau energy with the constraint that the sum of the volume fractions must stay equal to 1. The resulting model differs from the classical degenerate Cahn-Hilliard model (see [97], [77]) and is closely related to a model proposed by Weinan E and collaborators [76], [89]. Besides the derivation of the model, the convergence of a minimizing movement scheme is proven in [46].

#### 6.2. Calculus of variations applied to Image processing, physics and biology

In [23], Benoît Merlet et al. consider the branched transportation problem in dimension two with a cost of transport per unit length of path of the form  $f_a(m) = a + m$  where a > 0 is fixed and m is the flux along the path. As usual in branched transportation, an admissible transport is represented as a vector measure with prescribed divergence  $\sum m_j \delta_{x_j} - \sum m'_l \delta_{y_l}$  (the  $x_j$  representing the sources and the  $y_k$  the sinks). The paper introduces a family of functionals  $\{F_{\varepsilon}^a\}_{\varepsilon>0}$  and the authors establish that this family of functionals approximate the branched transportation energy in the sense of  $\Gamma$ -convergence. The energy  $F_{\varepsilon}^{a}$  is modeled on the Ambrosio-Tortorelli functional and is easy to optimize in practice (using dual formulation for the constraints and alternate direction optimization). In [48], the same authors extend their previous work to functionals defined on k-currents: the objects are no more lines that transport masses but k-dimensional surfaces transporting a given quantity of (k-1)-dimensional objects. The ambient space is now of any dimension n. A new family of approximate energies  $\{F_{\varepsilon}^a\}_{\varepsilon>0}$  is introduced and a  $\Gamma$ -convergence analysis is performed in the limit  $\varepsilon \downarrow 0$ . The limit objects are now k-currents with prescribed boundary, the limit functional controls both their masses (the total flux) and sizes (k-dimensional volume of the object). In the limit  $a \downarrow 0$ , the limit energy is the k-volume of the object so that these energies can be used for the numerical optimization of the size of k-currents with prescribed boundary. Although rather theoretical, the works [23], [48] are motivated by an image reconstruction issue: how to recover the contours of partially masked objects in an image.

In [26], Michael Goldman and Benoît Merlet study the strong segregation limit for mixtures of Bose-Einstein condensates modelled by a Gross-Pitaievskii functional. They study the behavior of minimizers of the Hamiltonian. First, they show that in the presence of a trapping potential, for different intracomponent strengths, the Thomas-Fermi limit is sufficient to determine the shape of the minimizers. Then they study the case of asymptotically equal intracomponent strengths: at leading order the two phases are then undistinguishable, the authors extract the next order and show that the relevant limit optimization problem is a weighted isoperimetric problem. Then, they study the minimizers, proving radial symmetry or symmetry breaking for different values of the parameters. Eventually, they show that in the absence of a confining potential, even for non-equal intracomponent strengths, one needs to study a related isoperimetric problem to gain information about the shape of the minimizers.
In [49], Michael Goldman, Benoît Merlet and Vincent Millot study a variational problem which models the behavior of topological singularities on the surface of a biological membrane in  $P_{\beta}$ -phase (see [92]). The problem combines features of the Ginzburg-Landau model in 2D and of the Mumford-Shah functional. As in the classical Ginzburg-Landau theory, a prescribed number of point vortices appear in the moderate energy regime; the model allows for discontinuities, and the energy penalizes their length. The novel phenomenon here is that the vortices have a fractional degree 1/m with m prescribed. Those vortices must be connected by line discontinuities to form clusters of total integer degrees. The vortices and line discontinuities are therefore coupled through a topological constraint. As in the Ginzburg-Landau model, the energy is parameterized by a small length scale  $\varepsilon > 0$ . The authors perform a complete  $\Gamma$ -convergence analysis of the model as  $\varepsilon \downarrow 0$  in the moderate energy regime. Then, they study the structure of minimizers of the limit problem. In particular, the line discontinuities of a minimizer solve a variant of the Steiner problem.

## 6.3. Asymptotic analysis for fluid mechanics

In [28], Ingrid Lacroix-Violet and Alexis 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.

In [44], the main objective is to generalize to the Navier-Stokes-Korteweg (with density dependent viscosities satisfying the BD relation) and Euler-Korteweg systems a recent relative entropy proposed in [65]. As a concrete application, this helps to justify mathematically the convergence between global weak solutions of the quantum Navier-Stokes system and dissipative solutions of the quantum Euler system when the viscosity coefficient tends to zero. Our results are based on the fact that Euler-Korteweg systems and corresponding Navier–Stokes-Korteweg systems can be reformulated through an augmented system. As a by-product of our analysis, we show that this augmented formulation helps to define relative entropy estimates for the Euler-Korteweg systems in a simplest way and with less hypothesis compared to recent works [74], [80].

In [27], Pierre-Emmanuel Jabin and Thomas Rey investigate the behavior of granular gases in the limit of small Knudsen number, that is, very frequent collisions. They deal with the strongly inelastic case in one dimension of space and velocity. They are able to prove the convergence toward 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. A more general result is also presented, which can apply to a large class of energy-dissipative kinetic equations.

## 6.4. Advanced discrete functional analysis results and applications

In [38], Claire Chainais-Hillairet, Benoît Merlet and Alexis Vasseur establish a positive lower bound for the numerical solutions of a stationary convection-diffusion equation on a bounded domain. The proof (which is fully detailed) is based on a celebrated method due to Ennio De Giorgi for showing regularity of the solutions of parabolic and elliptic equations. The robustness of the method allows the authors to adapt it to the discrete solutions obtained by standard finite volume discretizations. Further refinements of this work could lead to improve known error estimates for FV discretizations in  $L^p$ -norms to  $L^\infty$ -norm.

In [14], Marianne Bessemoulin-Chatard and Claire Chainais-Hillairet study the large-time behavior of a numerical scheme discretizing drift-diffusion systems for semiconductors. The numerical method is finite volume in space, implicit in time, and the numerical fluxes are a generalization of the classical Scharfet-ter-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  $L^{\infty}$  estimates for numerical solutions, which are then established in [35].

In [43], Marianne Bessemoulin-Chatard and Claire Chainais-Hillairet propose a new proof of existence of a solution to the scheme already introduced in [14] which does not require any assumption on the time step. The result relies on the application of a topological degree argument which is based on the positivity and on uniform-in-time upper bounds of the approximate densities. They also establish uniform-in-time lower bounds satisfied by the approximate densities. These uniform-in-time upper and lower bounds ensure the exponential decay of the scheme towards the thermal equilibrium as shown in [14].

In [12], Boris Andreianov, Clément Cancès, and Ayman Moussa developed a black box to obtain some compactness on the sequence produced by a finite volume discretization for degenerate parabolic problems. Such problems typically appear in the framework of porous media flows or in semi-conductor devices.

## 6.5. Structure preserving numerical methods

In [7], Clément Cancès and Cindy Guichard proposed in the case of a simple degenerate parabolic equation a nonlinear Control Volume Finite Element (CFVE) scheme that was able to preserve at the discrete level some important features of the continuous problem, namely the positivity of the solution, the decay of the physical energy. The scheme is based on a suitable upwinding procedure and inherits key properties from the Two-Point Flux Approximation (TPFA) finite volume scheme even though the method is not monotone. The convergence of the scheme towards the solution of the continuous problem was also established. In [22], Clément Cancès, Moustafa Ibrahim, and Mazen Saad extend the approach of [7] to the case of the Keller-Segel system with volume filling effect. In [11], Ahmed Ait Hammou Oulhaj, Clément Cancès, and Claire Chainais-Hillairet extend this approach to the Richards equation modeling unsaturated flow in porous media.

In presence of strong anisotropy, the methodology described above may lack robustness: the method is first order accurate, but the error constant may become large in some particularly unfavorable situations. This motivated the development of a new family of schemes with locally positive metric tensor (this denomination was chosen in reference Otto's contribution [90]). The methodology is first developed by Clément Cancès and Cindy Guichard for the so-called Vertex Approximate Gradient (VAG) scheme [79] in [21]. The newly developed method is second order accurate in space and much more robust with respect to the anisotropy than the one of [7] based on upwinding. Then Clément Cancès, Claire Chainais-Hillairet, and Stella Krell extend the methodology to Discrete Duality Finite Volume (DDFV) schemes in [32] and [19].

In [11] (see also the short version [31]), Ahmed Ait Hammou Oulhaj propose an upstream mobility TPFA finite volume scheme for solving a degenerate cross-diffusion problem modeling the flow of two fluids in a porous medium. The scheme has the remarkable property to preserve at the discrete level the local conservation of mass, the positivity of the solution, the decay of the energy. Moreover, the scheme provides a control on the entropy dissipation rate. Thanks to these properties, the convergence of the scheme is established. Numerical simulation show the great robustness of the scheme.

In [37], Clément Cancès and Flore Nabet propose an upstream mobility TPFA finite volume scheme for solving the degenerate Cahn-Hilliard problem. The scheme is designed in order to maintain the positivity of the phase volume fractions, the local conservation of mass and the decay of the energy.

Many applications involve partial differential equations which admits nontrivial steady state solutions. The design of schemes which are able to describe correctly these equilibrium states may be challenging for numerical methods, in particular for high order ones. In [29], inspired by micro-macro decomposition methods for kinetic equations, Lorenzo Pareschi and Thomas Rey 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.

## 6.6. Numerical approximation of a model for concrete carbonation

In [47], Claire Chainais-Hillairet, Benoît Merlet and Antoine Zurek introduce and study a finite volume scheme for a concrete carbonation model proposed by Aiki and Muntean in [55]. This model consists in a system of two weakly coupled parabolic equations in a varying domain whose length is governed by an ordinary

differential equation. The numerical scheme is obtained by a Euler discretization in time and a Scharfetter-Gummel discretization in space. The convergence of the scheme is established and the existence of a solution to the model is obtained as a by product. Finally, some numerical experiments are performed to show the efficiency of the scheme. The main results of this study are also concisely exposed in [34].

## 6.7. Numerical methods for stratigraphy problems

In the framework of the PhD thesis of Nicolas Peton, numerical methods are developed for nonlinear diffusion equations arising in stratigraphic modeling. In [33], the special case of a *p*-Laplacian equation with a constraint on the divergence of the flux is considered. Such a model is used to model erosion and sedimentation processes. The constraint is incorporated to take into account a maximal erosion rate.

## 6.8. Modeling and numerical simulation of complex fluids

In [25], Giacomo Dimarco, Raphaël Loub ere, Jacek Narski, and Thomas Rey extend the Fast Kinetic Scheme (FKS) 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 conservative 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.

In the context of the PhD of Claire Colin-Lecerf, C. Calgaro and co-authors derive in [45] a combined Finite Volumes - Finite Elements (CFVFE) scheme. This work can be seen as a generalization of some previous contributions on incompressible flows [5], [4], [6], in the context of a low-Mach model. Here, the temperature obeying an energy law has been taken into account. The authors chose to solve the continuity equation and the state equation linking temperature, density and thermodynamic pressure is imposed implicitly. Now the velocity field is no more divergence-free, so that the projection method solving the momentum equation has to be adapted. This combined scheme preserve the constant state and ensure the discrete maximum principle on the density. Their numerical results have been compared to some others which use purely finite elements schemes (see [62], [58], [81]) and in particular on a benchmark consisting in a transient hot jet entering in a cavity.

Diffuse interface models, such as the Kazhikhov-Smagulov model, allow to describe some phase transition phenomena. The theoretical analysis of this model was given by Bresch at al. [64] (see also reference therein). In the previous work [6], C. Calgaro et al. have implemented the CFVFE scheme and studied numerically the progression of the front of a powder-snow avalanche with respect to some characteristics parameters of the flow, such as the Froude, Schmidt and Reynolds numbers. In [18], C. Calgaro and co-authors investigate theoretically the CFVFE scheme. They construct a fully discrete numerical scheme for approximating the two-dimensional Kazhikhov-Smagulov model, using a first-order time discretization and a splitting in time to allow the construction of the combined scheme. Consequently, at each time step, one only needs to solve two decoupled problems, the first one for the density (using the Finite Volume method) and the second one for the velocity and pressure (using the Finite Element method). The authors prove the stability of the combined scheme and the convergence towards the global in time weak solution of the model. In this model, the convection-diffusion equation for the density can also be discretized by a implicit-explicit (IMEX) second order method in the Finite Volume scheme. In the framework of MUSCL methods, C. Calgaro and M. Ezzoug prove in [36] that the local maximum property is guaranteed under an explicit Courant-Friedrichs-Levy condition and the classical hypothesis for the triangulation of the domain.

## 6.9. Cost reduction of numerical methods

This section gathers contributions for which the main motivation was to increase the efficiency of numerical methods, either by localizing the computational effort thanks to mesh refinement

In [24], E. Creusé and his collaborators generalize the equilibrated error estimators developed in the lowfrequency magnetostatic case to the case of the harmonic time-dependent one. This contribution allows to obtain a bound of the numerical error equal to one, so that the accuracy of the obtained solution can be explicitly controlled.

The contribution [16] 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 [16], 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 [16] 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 a strong robustness of the method w.r.t. the nonlinearities appearing in the continuous model.

In [39], Ward Melis, Thomas Rey, and Giovanni Samaey present a high-order, fully explicit, asymptoticpreserving projective integration scheme for the nonlinear BGK equation. The method first takes a few small (inner) steps with a simple, explicit method (such as direct forward Euler) to damp out the stiff components of the solution. Then, the time derivative is estimated and used in an (outer) Runge-Kutta method of arbitrary order. Based on the spectrum of the linearized BGK operator, they deduce that, with an appropriate choice of inner step size, the time step restriction on the outer time step as well as the number of inner time steps is independent of the stiffness of the BGK source term. They illustrate the method with numerical results in one and two spatial dimensions.

In [13], Christophe Besse, Guillaume Dujardin, and Ingrid Lacroix-Violet present the numerical integration in time of nonlinear Schrödinger equations with rotating term. After performing a change of unknown so that the rotation term disappears they consider exponential integrators such as exponential Runge-Kutta methods and Lawson methods. They provide an analysis of the order of convergence and some preservation properties of these methods and they present numerical experiments.

## **APICS Project-Team**

## 5. New Results

## 5.1. Inverse problems for Poisson-Laplace equations

**Participants:** Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Jean-Paul Marmorat, Konstantinos Mavreas, Christos Papageorgakis.

#### 5.1.1. Inverse magnetization issues from planar data

This work is carried out in the framework of the Inria Associate Team IMPINGE, comprising Cauê Borlina, Eduardo Andrade Lima and Benjamin Weiss from the Earth Sciences department at MIT (Boston, USA) and Douglas Hardin, 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). Depending on the nature of the rock sample, the magnetization distribution can either be considered to lie in a plane or in a parallelepiped of thickness r. Some of our results apply to both frameworks (the former appears as a limiting case when r goes to 0), while others concern the 2D case and have no 3-D counterpart yet.



Figure 3. Schematic view of the experimental setup

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 pursued this year our research efforts towards designing algorithms for net moment recovery. The net moment is the integral of the magnetization over its support, and it is a valuable piece of information to physicists which has the advantage of being determined solely by the field: whereas two different magnetizations can generate the same field, the net moment depends only on the field and not on which magnetization produced it. Hence the goal may be described as to build 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 using the fact that the integral of  $B_3$  against polynomials of order less or equal to 1 on some domains symmetric with respect to the origin provides an estimate of the net moment, asymptotically when R grows large [34]. This approach was tested this year on real data measured with the SQUID microscope at MIT. Applying directly the formulas on the measured data led to poor results, and we identified this issue as a consequence of electronic noise (drift of the measured field). This noise was impeding the method, especially when R was large, preventing one from getting estimates of the net moment with an error smaller than about 10%. By modeling this fairly deterministic drift as an affine function of the space variables, we were able to pretty much cancel out its effect. With this correction, the curve obtained when R varies follows fairly accurately the theoretical asymptotic behavior. We fit this curve with the one corresponding to the theoretical behavior, which allows us to extrapolate its value at infinity, hence giving us an estimate of the net moment. The results on some experimental data (chondrules) are promising. Yet, results on some other data sets are still unsatisfactory and remain to be understood.

The second approach attempts to generalize the previous expansions in the case when R is moderately large. This work is carried out in the thin slab framework, modeling the sample as a rectangle. Last year, we set up a bounded extremal problem (BEP, see Section 3.3.1) consisting in finding the functions  $\phi_i$  (i = 1, 2, 3) such that  $|\langle m_i \rangle - \iint \phi_i(x_1, x_2) B_3(x_1, x_2) dx_1 dx_2|$  is least possible under the constraint that  $||\nabla \phi_i||_2 \leq M$ , where M is a user-defined parameter. This year, we sharpened our regularity results on the solutions with respect to space variables and the parameters of the problem (*e.g.*, the level of constraint M), and considered several resolution schemes. We implemented an algorithm approximately solving for the critical point equation, using a finite elements method. Numerical experiments on synthetic data confirm the validity of the approach with small noise, see [21]. The addition of a synthetic noise, however, has revealed sensitivity to a poor signal / noise ratio, in particular at measurement points close to the edges of the measurement slab where the estimator oscillates heavily. Such oscillations are the price to pay for an estimation procedure which uses data on a measurement set not much bigger than the sample. This is an interesting feature of the method, and further analysis is needed to offset the noise effect. Notice that the work [21] also includes 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 started this year to design an alternate procedure to compute a good linear estimator. It consists in expanding it on a family of piecewise affine functions, with a restricted number of pieces. This still needs 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. On a related topic, we also derived explicit formulas for the adjoint operator  $B_3^*$  to  $B_3$  (in appropriate  $L^2$  spaces), when applied to polynomials. This adjoint operator is central to the construction of linear estimators, and these formulas suggest one could work efficiently with polynomial bases. This work is still in progress.

Concerning full inversion of thin samples, after preliminary experiments on regularization with  $L^1$  constraints (a heavy trend in linear inverse problems today to favor sparse solutions), we started studying magnetizations modeled by signed measures. A loop decomposition of silent sources was obtained, which makes precise in the 2-D setting the structure theorem of [78]. Moreover, a characterization of equivalent sources having minimal total variation has been obtained when the support of the magnetization is very scattered (purely 1unrectifiable, which holds in particular for dipolar models) and also for certain magnetizations of geophysical interest like unidirectional ones. Thus, it seems that constraining the total variation to regularize the recovery process is appropriate in some important cases. The theoretical analysis has shown that the optimum is then always sparse, in that it has Hausdorff dimension at most 1. This stems from the real analyticity of operators relating the magnetization to the field, which prevents them from assuming constant level on large sets. An implementation is currently being set up with promising results. Yet, a deeper understanding on how to adjust the parameters of the method is required. This topic is studied in collaboration with D. Hardin and C. Villalobos from Vanderbilt University.

Besides, we considered a simplified 2-D setup for magnetizations and magnetic potentials (of which the magnetic field is the gradient). When both the sample and the measurement set are parallel intervals, some best approximation issues related to inverse recovery and relevant BEP problems in Hardy classes of holomorphic functions (see Section 3.3.1) were solved in [19]. Note that, in the present case, the criterion no longer acts on the boundary of the holomorphy domain (namely, the upper half-plane), but on a strict subset thereof, while the constraint acts on the support of the approximating function. Both involve real parts of functions in the Hilbert Hardy space of the upper half-plane. This is joint work with D. Ponomarev (see Section 7.5.1). Some extensions are the subject of ongoing work with E. Pozzi (Department of Mathematics and Statistics, St Louis Univ., St Louis, Missouri, USA). They concern more precise approximation criteria, and the development of resolution schemes using the Fourier basis. Meanwhile, BEP in Bergman classes of analytic or generalized analytic functions are under being studied with B. Delgado Lopez (see Section 3.2, 7.5.1).

For magnetizations supported in a volume  $\Omega$  with boundary  $\partial\Omega$ , there is a greater variety of silent sources, since they have much more space to live in. Now, to each magnetization m supported in  $\Omega$  there is a unique magnetization supported on  $\partial\Omega$  (the balayage of m) and producing the same field outside  $\Omega$ . Thus, describing silent sources supported on  $\partial\Omega$  is a way to factor out some of the complexity of the situation. When mis located in the plane, the Hardy-Hodge decomposition introduced in [38] (see Section 3.3.1) was used there to characterize all silent magnetizations from above (resp.below) as being those having no harmonic gradient from below (rep. above) in their decomposition. When m is supported on a compact surface, a similar decomposition exists for  $\mathbb{R}^3$ -valued vector fields on  $\partial\Omega$ , (see Section 5.4), that allows to characterize all magnetizations on  $\partial\Omega$  which are silent from outside as being those whose harmonic components satisfy a certain spectral relation for the double layer potential on  $\partial\Omega$ . The analysis and the algorithmic use of that equation for recovery or moment estimation remain to be worked out.

Other types of inverse magnetization problems can be tackled using such techniques, in particular global Geomagnetic issues which arise in spherical geometry. This year, in collaboration with C. Gerhards from the University of Vienna (Austria), we developed a method to separate the crustal component of the Earth's magnetic field from its core component, if an estimate of the field is known on a subregion of the globe [23]. This assumption is not unrealistic: parts of Australia and of northern Europe are considered as fairly well understood from the magnetostatic view point. We look forward to test the algorithm against real data, in collaboration with Geophysicists

#### 5.1.2. Inverse magnetization issues from sparse cylindrical 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 think that the Moon used to have a magnetic dynamo for a while. However, 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 a couple of times 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  $B_{\tau}$  tangential to the circle (red points).

This year, we continued the approach taken in previous years. Under the hypothesis that the field can be well explained by a single magnetic pointwise dipole, and using ideas similar to those underlying the FindSources3D tool (see Sections 3.4.2 and 5.1.3), we try to recover the position and the moment of the dipole using the available measurements.

In a given cylinder, using the associated cylindrical system of coordinates, recovering the position of the dipole boils down to determine its height z, its radial distance  $\rho$  and its azimuth  $\phi$ . In principle, the rational approximation technique that we are using returns, for the circle of measurements at height h, the unique complex pole  $\xi_h$  of order five belonging to the corresponding normalized disk of some rational function. From this pole, the complex number  $u_h = \xi_h + \frac{1}{\xi_h} = \frac{1+\rho^2+(h-z)^2}{\rho} e^{i\phi}$  can be estimated. 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, only an approximation of  $u_h$  is computed. The question is then to reliably combine the information provided by all circles of measurements, in order to recover z,  $\rho$  and  $\phi$ . The azimuth is fairly easy to obtain: we can estimate it, *e.g.*, by taking the mean value of the argument of  $\xi_h$ , for all h for which we have a measurement circle, possibly excluding one of them when the provided estimate seems to be clearly different from the others. As regards the reconstruction of  $\rho$  and z, we designed this year two new strategies.

The first strategy consists in observing that  $\rho |u_h| = 1 + \rho^2 + h^2 - 2hz + z^2$ , whence doing the difference with the same equation obtained at height  $h': \rho (|u_h| - |u_{h'}|) = (h^2 - h'^2) - 2(h - h')z$ . This provides a linear relation between the unknowns  $\rho$  and z. Three measurement circles provide us with two independent relations and are in principle enough to recover  $\rho$  and z. Numerical experiments showed that this recovery strategy is unsatisfactory: it is fairly sensitive to approximation errors on the estimates  $|u_h|$  and  $|u_{h'}|$ , hence the estimation procedure is unstable. However, it might become more robust if data were available on more than three circles per cylinder. Exploring this idea is an on-going piece of work. If successful, it will suggest an easy modification of the magnetometer of Cerege for future measurements campaigns.

The second strategy directly uses the pole  $\xi_h$  instead of  $u_h$ , hence avoiding numerical steps that are possible sources of errors. It consists in observing that  $|\xi_h|$  is maximal, with respect to h, when h = z and it is then equal to  $\rho e^{i\phi}$ . A rough estimate of  $\rho$  is hence given by the maximal value of  $|\xi_h|$  among the three values of havailable for each cylinder. The position of the dipolar source is then estimated by combining the estimates of  $\rho$  and  $\phi$  obtained on all three cylinders. The moment is then computed from this estimated position, solving a linear system by least-squares techniques. Although not sophisticated, this method gave promising results on synthetic examples, with more or less noise, see the submitted work [25]. This is still on-going work which constitutes the main topic of the PhD thesis of K. Mavreas.

#### 5.1.3. Inverse problems in medical imaging

This work is conducted in collaboration with Maureen Clerc and Théo Papadopoulo, from the team Athena (Inria Sophia).

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], [43] 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 (FS3D, see Section 3.4.2) is being developed, in collaboration with the Inria team Athena and the CMA - Mines ParisTech. In addition to the modular and ergonomic platform version of FS3D, 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 that correspond to measurements of the electrical potential, one should consider *triple* poles; for (magnetic) field data however, like in Section 5.1.2 or from MEG – magneto-encephalography –

data, one should consider poles of order five). 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, the version of the software currently under development takes as inputs actual EEG measurements, like time signals, and performs a suitable singular value decomposition in order to separate independent sources.

Magnetic data from MEG recently became available along with EEG data, by our medical partners at the hospital la Timone; indeed, it is now possible to use simultaneously both measurement devices, in order to measure both the electrical potential and a component of the magnetic fields. This should enhance the accuracy of our source recovery algorithms. We will add the treatment of MEG data as another functionality of the software FS3D.

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 Inria team Athena and BESA GmbH, see Section 6.1.2). In layered models, it concerns the estimation of the conductivity of the skull (an intermediate layer). First, the conductivity of the skull can differ from one individual to another, or for the same person, along the time, and is much smaller than those of the surrounding layers (the brain and the scalp). A preliminary issue in this direction was to estimate a single-valued skull conductivity from one EEG recording. Existence, uniqueness, stability properties and a recovery scheme for this conductivity value were established in the spherical setting when the sources are known, see [10]. When the sources are unknown, we must look for additional data (additional clinical and/or functional EEG, EIT, ...) that could be incorporated in order to recover both the sources locations and the skull conductivity. Second, 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 actually possess quite different conductivities. The influence of the second on the overall model is also studied in [10], together with a numerical process allowing to estimate the hard bone conductivity value together with a dipolar source, in realistic geometries.

We also began to consider the inverse problem of recovering the parameters of a skin tumor from thermal measurements, in a 2-D model that takes the form of a static Schrödinger equation. This is joint work with F. Ferranti (IMT Atlantique, Microwave Department) and the topic of the internship of G. Dervaux, see Section 7.5.1.

## 5.2. Matching problems and their applications

Participants: Laurent Baratchart, Martine Olivi, Gibin Bose, 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) as well as with, Fabien Ferrero (LEAT, Sophia-Antipolis, France) Leonardo Lizzi (LEAT, Sophia-Antipolis, France).

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. Filter plugged on a system with reflection coefficient  $L_{11}$ 

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:

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

The matching problem of minimizing  $|G_{1,1}|$  amounts therefore to minimize the pseudo-hyperbolic distance  $\delta$  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 nfrequency 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  $\psi(p) = (p/q(x_1), \dots, p/q(x_n))$ is a homeomorphism from monic polynomials of degree n onto  $\mathbb{D}^n$  ( $\mathbb{D}$  the complex open disk), and  $\psi^{-1}$  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. The detailed mathematical proofs can be found in [11].

#### 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. It can 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 are quite convincing, we have no proof of their global optimality. This has led us to seek alternative approaches allowing us to assess, at least in simple cases, global optimality of the obtained response. By optimality of a response we mean, as in classical filtering, a best match of the response in the uniform norm on a given pass-band, while meeting given rejection constraints on a stop-band. Following the approach of Fano and Youla, we considered the problem of designing a  $2 \times 2$  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, 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 in degree 1), it is therefore possible to perform filter synthesis with a guarantee on the global optimality of the obtained characteristics. The constructive aspects of this approach, relying on convex duality and linear programming, were presented in [16], together with an implementation using a SIW (substrate integrated filter). For antennas with a transmission coefficient of higher degree, like dual band antennas, we developed a convex relaxation of the matching problem which yields a set lower bounds on the matching error, for every considered degree of the overall system (matching system + load). This substantially improves Helton's approach, that furnishes a single global theoretical lower bound independent of the degree, obtained via an infinite degree  $H^{\infty}$  relaxation of the problem. A preliminary version of this approach was presented in [15], while a more detailed paper is under way. We consider this to be an important breakthrough concerning this classical problem in electronics. The implementation of the method involves solving a convex optimization problem on the cone of positive polynomials under some non-linear, yet convex, matrix inequality constraints. Solving the latter combining logarithmic barrier functions and Lagrangian relaxation techniques provided us, for example, with an excellent initial design for a matching network dedicated to an array of dual-band antennas with circular polarization, studied in the context of the ANR Cocoram. Design of matching networks for complex antennas is also considered in collaboration with LEAT, within the context of Gibin's Bose PhD.

## 5.3. Stability assessment of microwave amplifiers and design of oscillators

**Participants:** Laurent Baratchart, Sylvain Chevillard, Martine Olivi, Fabien Seyfert, Sébastien Fueyo, Adam Cooman.

The goal is here 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 (S. Fueyo) and a postdoctoral (A. Cooman) student along with planned software developments. Application of our work to oscillator design methodologies started recently with Smain Amari from the Royal Military College of Canada (Kingston, Canada).

As opposed to Filters and Antennas, Amplifiers and Oscillators are active components that intrinsically entail a non-linear functioning. The latter is due to the use of transistors governed by electric laws exhibiting saturation effects, and therefore inducing input/output characteristics that are no longer proportional to the magnitude of the input signal. Hence they typically produce non-linear distortions. A central question arising in the design of amplifiers is to assess stability. The latter may be understood around a functioning point when no input but noise is considered, or else around a periodic trajectory when an input signal at a specified frequency is applied. For oscillators, a precise estimation of their oscillating frequency is crucial during the design process. As regards devices devised to operate at relative low frequencies, time domain simulations, based on the integration of the underlying non-linear dynamical system, answers these questions satisfactorily. For complex microwave amplifiers and oscillators, the situation is however drastically different: the time step necessary to integrate the transmission line's dynamical equations (which behave like simple electrical wire at low frequency) becomes so small that simulations are intractable in reasonable time. In addition to this problem, most linear components of these circuits are known through their frequency response, and require therefore a preliminary, numerically unstable step to obtain their impulse response, prior to any time domain simulation.

For all these reasons it is widely preferred to perform the analysis of such systems in the frequency domain. In the case of stability issues around a functioning point, where only small input signals are considered, the stability of the linearized system obtained by a first order approximation of each non-linear dynamic is considered. This is done by means of the analysis of transfer impedance functions computed at some ports of the circuit. We have shown, that under some realistic hypothesis on the building blocks of the circuit, these transfer functions are meromorphic functions of the frequency variable s, with at most a finite number of unstable poles in the right half-plane [20]. Dwelling on the unstable/stable decomposition in Hardy Spaces, we developed a procedure to assess the stability or instability of the transfer functions at hand, from their evaluation on a finite frequency grid [12]. The data are generally supplied by circuit simulators, used by microwave device designers. We are currently working towards precise estimation techniques of the unstable poles of these transfer functions, hence on the evaluation of their rational unstable part. Our approach involves here the AAK theory, furnishing at low cost a rough estimate of the desired singularities, combined with specialized versions of stable rational approximation procedures. Practical application of this work are sought among the microwave amplifier design community as well as for the synthesis of oscillators: for the latter, a precise location of one unstable poles is necessary. A software toolbox is being developed for this purposes, and a collaboration on this project has started with Smain Amari from the Royal Military College on microwave oscillator design.

When stability is studied around a periodic trajectory, which is determined in practice by Harmonic Balance algorithms, linearization yields a linear time varying dynamical system with periodic coefficients and a periodic trajectory thereof. While in finite dimension the stability of such systems is well understood via the Floquet theory, this is no longer the case in the infinite dimensional setting when delays are considered. Dwelling on the theory of retarded systems, S. Fueyo's PhD work has made remarkable progress on this topic by showing that, for certain simple circuits with properly positioned resistors, the monodromy operator is a compact perturbation of a stable operator, and that only finitely many unstable point of its spectrum can occur. A practical application of this result is to generalize the previously described techniques of stability assessment around a functioning point into a stability assessment technique around periodic trajectories. This can be recast in terms of the finiteness of the number of abscissas of unstable poles of the Harmonic Transfer functions of the circuit. It will be of great importance to generalize such considerations to more complex circuits, whose structure is less well understood at present.

## 5.4. The Hardy-Hodge decomposition

#### Participant: Laurent Baratchart.

(This is joint work with Qian T. and Dang P. from the university of Macao.) It was proven in previous year that on a smooth compact hypersurface  $\Sigma$  embedded in  $\mathbb{R}^n$ , a  $\mathbb{R}^n$ -valued vector field of  $L^p$  class decomposes as the sum of a harmonic gradient from inside  $\Sigma$ , a harmonic gradient from outside  $\Sigma$ , and a tangent divergence-free field. This year we extended this result to Lipschitz surfaces for  $2 - \varepsilon , where <math>\varepsilon$  and  $\varepsilon'$  depend on the Lipschitz constant of the surface. We also proved that the decomposition is valid for  $1 when <math>\Sigma$  is VMO-smooth (*i.e.*  $\Sigma$  is locally the graph of Lipschitz function with derivatives in VMO). By projection onto the tangent space, this gives a Hodge decomposition for 1-forms on a Lipschitz surface, which is apparently also new since existing results deal with smooth surfaces (but forms of any degree). This result was reported at the invited session on Harmonic Analysis and Inverse Problems of the Mathematical Congress of the Americas, an article is being written to report on it.

## **BIPOP Project-Team**

## 7. New Results

## 7.1. 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. 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 [24]. It relies on a particular limiting process of normal cones.

## 7.2. Discrete-time sliding mode control

Participants: Vincent Acary, Bernard Brogliato.

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  $h^2$ . 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. In particular the high frequency bangbang 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 [48]. The previous results deal with disturbances which are matched and uniformly upperbounded. In [26] the SMC of Lagrange systems is studied. In [35] this is 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. A nested controller is proposed in [36], using a backstepping-like approach for the controller synthesis.

## 7.3. Linear Complementarity Systems

Participants: Bernard Brogliato, Christophe Prieur, Alexandre Vieira.

The quadratic optimal control of Linear complementarity systems (LCS) is analysed in [37]. The major difficulty comes from the fact that complementarity conditions introduce non convex constraints. Suitable algorithms have to be used to solve the MPEC problems for solving the direct method. The indirect (Pontryagin's) approach is quite delicate and is currently analysed in the PhD thesis of A. Vieira.

## 7.4. 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.

#### 7.4.1. Numerical time-integration methods for event-detecting schemes.

Participants: Vincent Acary, Bernard Brogliato.

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  $\alpha$ -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. The results are reported in [23].

#### 7.4.2. Multibody systems with clearances (dynamic backlash)

Participants: Vincent Acary, Bernard Brogliato.

The PhD thesis of N. Akadkhar under contract with Schneider Electric has concerned 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. Circuits breakers with 3D joint clearances have been studied in [20], [31] where it is demonstrated that the nonsmooth dynamics approach as coded in our software SICONOS, allows a very good prediction of the system's dynamics, with experimental validation. An overview of various approaches for the feedback control of multibody systems with joint clearances is proposed in [21].

## 7.5. Nonlinear waves in dissipative granular chains

Participants: Guillaume James, Bernard Brogliato, Kirill Vorotnikov.

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. In order to describe the response of such systems to impacts or vibrations, it is important to analyze different wave effects such as the propagation of localized compression pulses (solitary waves) or the scattering of vibrations through the chain. Such phenomena are strongly influenced by contact nonlinearities (Hertz force), spatial inhomogeneities and dissipation. In this work, we analyze the Kuwabara-Kono (KK) model for contact damping, and we develop new approximations of this model which are efficient for the simulation of multiple impacts. The KK model is a simplified viscoelastic contact model derived from continuum mechanics, which allows for simpler calibration (using material parameters instead of phenomenological ones), but its numerical simulation requires a careful treatment due to its non-Lipschitzian character. Using different dissipative time-discretizations of the conservative Hertz model, we show that numerical dissipation can be tuned properly in order to reproduce the physical dissipation of the KK model and associated wave effects. This result is obtained analytically in the limit of small time steps (using methods from backward analysis) and is numerically validated for larger time steps. The resulting schemes turn out to provide good approximations of impact propagation even for relatively large time steps.

## 7.6. Periodic motions of coupled impact oscillators

Participants: Guillaume James, Vincent Acary, Franck Pérignon.

In the work [40], we study the existence and stability of time-periodic oscillations in an infinite chain of linearly coupled impact oscillators, for rigid impacts without energy dissipation. We reformulate the search of periodic solutions as a boundary value problem incorporating unilateral constraints. This formulation, together with an appropriate notion of nondegenerate modes, allows us to construct nonsmooth modes of oscillations (spatially localized or extended) when the oscillators are weakly coupled (this approach is an adaptation of the idea of "anticontinuum" limit to the nonsmooth setting). In this framework, we show the existence of exact solutions (in particular, we check the condition of non-penetration of the obstacle) for an arbitrary number of impacting particles. Different solution branches corresponding to stable or unstable breathers, multibreathers and nonsmooth normal modes are found. We provide a formula for the monodromy matrix that determines spectral stability of nonsmooth modes in the presence of simple impacts. These results are completed by a numerical computation of the time-periodic solutions at larger coupling, and the Siconos software is used to simulate the system and explore dynamical instabilities. The above approach is much more effective than numerical continuation of periodic solutions based on stiff compliant models, which leads to stiff ODEs and costly numerical continuation.

## 7.7. Stability analysis for rogue waves

## Participant: Guillaume James.

The study of rogue waves (large amplitude waves localized both in space and time) has gained importance in various fields, such as the mathematical modeling of water waves and nonlinear optics. The analysis of their stability is delicate because of their transient nature. In the work [46], we introduce a new method to tackle this problem. Our approach relies on the approximation of rogue waves by large amplitude breathers (localized in space and time-periodic) having a large period, and the use of Floquet theory to analyze breather stability. This problem is examined for the nonlinear Schrödinger equation, which describes the envelope of nonlinear waves in a large class of systems, for example granular chains [15]. This model admits a family of breather solutions (Kuznetsov-Ma breathers) which converge to a rogue-wave profile (Peregrine soliton) when their period tends to infinity. We show numerically that the Floquet exponents of the breathers approach a finite limit for large periods, and observe that a motion of the localized wave can be induced by a dynamical instability. This work suggests an analytical way to define the spectral stability of the (transient) Peregrine soliton, but this remains an open problem to prove analytically the convergence of Floquet exponents in the limit of infinite period.

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

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

Spatially discrete systems (lattice differential equations) have a wide range of applications in natural sciences, engineering and social sciences. They frequently occur in physics as mass-spring systems with nearest-neighbors coupling and they have been used extensively to describe the dynamics of microscopic structures such as crystals or micromechanical systems, or to model fragmentation phenomena.

In this work, we consider a spring-block system that slides down a slope due to gravity. Each block is subjected to a nonlinear friction force. This system differs from the Burridge-Knopoff model considered for the modeling of earthquakes, which incorporates local potentials. We perform numerical simulations of the coupled system and show that the bistability property induces traveling patterns, as fronts and pulses. 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 published in [27].

## 7.9. 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. 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. These results have been reported in [28].

We have obtained an existence theorem for solitary waves in the Burridge-Knopoff model. Our approach uses a piecewise-linear friction force combined with a weak coupling strength. Using asymptotic arguments, we show that trial solutions, obtained semi-analytically, satisfy, for some parameter set, the inequality constraints associated with the threshold conditions. An approximation of the wave profile is obtained and a minimal wave speed is derived.

## 7.10. Propagation in space-discrete excitable systems

Participant: Arnaud Tonnelier.

We introduce a simplified model of excitable media where the response of an isolated element to an incoming signal is given by a fixed pulse-shape function. When the total activity of one element reaches a given threshold, a signal is sent to its N nearest neighbors. We show that an excitable chain supports the propagation of a set of simple traveling waves where the interval between the emitting time of two successive elements remains constant. We propose a classification of travelling waves that depends on the number of signals that are received by an element. Results on stability of travelling signals are derived. We also discussed the global shape of the speed curve (velocity of the wave with respect to the global coupling strength). In particular, we show that for a given network connectivity, different wave velocities can be obtained, i.e., depending on initial conditions, the network may propagate different signals. A comprehensive study is done for a transmission line with N = 2 and N = 3. Some necessary conditions for multistationarity are derived for an arbitrary N and for different network connectivities.

## 7.11. Inverse design of a suspended elastic rod

Participants: Florence Bertails-Descoubes, Victor Romero.

In collaboration with Alexandre Derouet-Jourdan (OLM Digital, Japan) and Arnaud Lazarus (UPMC, Laboratoire Jean le Rond d'Alembert), we have investigated the inverse design problem of a suspended elastic subject to gravity. We have proved that given an arbitrary space curve, there exists a unique solution for the natural configuration of the rod, which is independent of the initial framing of the input curve. Moreover, this natural configuration can be easily computed by solving three linear ODEs in sequence, starting from any input framing. This work has just been submitted for publication in physics.

## 7.12. Simulation of cloth contact with exact Coulomb friction

Participant: Florence Bertails-Descoubes.

In collaboration with Gilles Daviet (Weta Digital, New Zealand), Rahul Narain and Jie Lie (University of Minnesota), we have developed a new implicit solver for taking into account contact in cloth with Coulomb friction. Our key idea stems from the observation that for a nodal system like cloth, and in the case where each node is subject to at most one contacting constraint (either an external or self-contact), the frictional contact problem may be formulated based on velocities as primary variables, without having to compute the costly Delassus operator; then, by reversing the roles classically played by the velocities and the contact impulses, conical complementarity solvers of the literature may be leveraged to solve for compatible velocities at nodes. To handle the full complexity of cloth dynamics scenarios, we have extended this base algorithm in two ways: first, towards the accurate treatment of frictional contact at any location of the cloth, through an adaptive node refinement strategy; second, towards the handling of multiple constraints at each node, through the duplication of constrained nodes and the adding of pin constraints between duplicata. Our method proves to be both fast

and robust, allowing us to simulate full-size garments with more realistic body-cloth interactions compared to former methods, while maintaining similar computational timings. Our work will be submitted for publication to Siggraph 2018.

## 7.13. Model Predictive Control for biped walking motion generation

**Participants:** Pierre-Brice Wieber, Nestor Alonso Bohorquez Dorante, Nahuel Villa, Matteo Ciocca, Stanislas Brossette, Alexander Sherikov.

We proposed last year a feasible Newton scheme for nonlinear MPC by combining ideas from robust control and trust regions. This year, we applied this approach to nonlinearities that appear when adapting step durations [32]. We also investigated more thoroughly the strong recursive feasibility of our scheme [34] and how it could be adapted to situations with bounded uncertainty [29]. Finally, we proposed a new approach to collision avoidance based on separating planes [38].

## **COMMANDS Project-Team**

## 7. New Results

## 7.1. Deterministic Optimal Control

#### 7.1.1. Galerkin approximations of nonlinear optimal control problems in Hilbert spaces Participant: Axel Kroner.

With Mickaël D. Chekroun (UCLA), and Honghu Liu (Virginia Tech). Nonlinear optimal control problems in Hilbert spaces are considered for which we derive approximation theorems for Galerkin approximations. Approximation theorems are available in the literature. The originality of our approach relies on the identification of a set of natural assumptions that allows us to deal with a broad class of nonlinear evolution equations and cost functionals for which we derive convergence of the value functions associated with the optimal control problem of the Galerkin approximations. This convergence result holds for a broad class of nonlinear control strategies as well. In particular, we show that the framework applies to the optimal control of semilinear heat equations posed on a general compact manifold without boundary. The framework is then shown to apply to geoengineering and mitigation of greenhouse gas emissions formulated for the first time in terms of optimal control of energy balance climate models posed on the sphere  $S^2$ . See [12].

# 7.1.2. Galerkin approximations for the optimal control of nonlinear delay differential equations

Participant: Axel Kroner.

With Mickaël D. Chekroun (UCLA), and Honghu Liu (Virginia Tech).

Optimal control problems of nonlinear delay differential equations (DDEs) are considered for which we propose a general Galerkin approximation scheme built from Koornwinder polynomials. Error estimates for the resulting Galerkin-Koornwinder approximations to the optimal control and the value function, are derived for a broad class of cost function-als and nonlinear DDEs. The approach is illustrated on a delayed logistic equation set not far away from its Hopf bifurcation point in the parameter space. In this case, we show that low-dimensional controls for a standard quadratic cost functional can be efficiently computed from Galerkin-Koornwinder approximations to reduce at a nearly optimal cost the oscillation amplitude displayed by the DDE's solution. Optimal controls computed from the Pontryagin's maximum principle (PMP) and the Hamilton-Jacobi-Bellman equation (HJB) associated with the corresponding ODE systems, are shown to provide numerical solutions in good agreement. It is finally argued that the value function computed from the corresponding reduced HJB equation provides a good approximation of that obtained from the full HJB equation. See [16].

## 7.2. Stochastic Control

## 7.2.1. On the time discretization of stochastic optimal control problems: the dynamic programming approach

Participant: Frederic Bonnans.

With Justina Gianatti (U. Rosario) and Francisco J. Silva (U. Limoges) In this work we consider the time discretization of stochastic optimal control problems. Under general assumptions on the data, we prove the convergence of the value functions associated with the discrete time problems to the value function of the original problem. Moreover, we prove that any sequence of optimal solutions of discrete problems is minimizing for the continuous one. As a consequence of the Dynamic Programming Principle for the discrete problems, the minimizing sequence can be taken in discrete time feedback form. See [17].

#### 7.2.2. Variational analysis for options with stochastic volatility and multiple factors

Participants: Frederic Bonnans, Axel Kroner.

We perform a variational analysis for a class of European or American options with stochastic volatility models, including those of Heston and Achdou-Tchou. Taking into account partial correlations and the presence of multiple factors, we obtain the well-posedness of the related partial differential equations, in some weighted Sobolev spaces. This involves a generalization of the commutator analysis introduced by Achdou and Tchou. See [18].

## 7.2.3. Infinite Horizon Stochastic Optimal Control Problems with Running Maximum Cost Participant: Axel Kroner.

With Athena Picarelli (U. Oxford) and Hasna Zidani (ENSTA).

An infinite horizon stochastic optimal control problem with running maximum cost is considered. The value function is characterized as the viscosity solution of a second-order HJB equation with mixed boundary condition. A general numerical scheme is proposed and convergence is established under the assumptions of consistency, monotonicity and stability of the scheme. A convergent semi-Lagrangian scheme is presented in detail. See [19].

## 7.3. Applications

## 7.3.1. On the Design of Optimal Health Insurance Contracts under Ex Post Moral Hazard Participant: Pierre Martinon.

With Pierre Picard and Anasuya Raj (Ecole Polytechnique, Econ. dpt).

We analyze in [20] 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-off 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 insurers rates are affected 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. Numerical simulations indicate that these qualitative results tend to be robust with respect to the health parameter.

## **DISCO Project-Team**

## 7. New Results

## 7.1. Maximal-multiplicity-based rightmost-root assignment for retarded TDS

**Participants:** Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S], Hakki Unal [Anadolu University], Toma Vyhlidal [Czech Technical University].

The proposed approach is a stabilizing delayed state-feedback design guaranteeing an appropriate (admissible) convergence rate to the trivial solution of the controlled dynamical system. Unlike methods based on finite spectrum assignment, our method does not render the closed loop system finite dimensional but consists in controlling its rightmost spectral value. First, it consists in characterizing the root of the characteristic quasipolynomial function to be of maximal multiplicity by mean of an analytical necessary and sufficient condition. Then, conditions on such a root (of maximal multiplicity) to be stable and dominant are established. These results are obtained for reduced-orders time-delay system (scalar and quadratic cases), see [69].

## 7.2. Migration of multiple roots under parameters/delays perturbation

Participants: Islam Boussaada, Dina Irofti, Silviu-Iulian Niculescu, Wim Michiels [KU Leuven].

In the context of the perturbation theory of nonlinear eigenvalue problem, the sensitivity of multiple eigenvalues with respect to parameters' variations is studied. In the complete regular splitting case, explicit expressions for the leading coefficients of the Puiseux series of the eigenvalue are provided [22]. In contrast to existing analysis of multiple roots of delay equations the developed results are in a matrix framework, i.e., without reduction of the problem to the analysis of a scalar characteristic quasipolynomial.

## 7.3. A generalized $\tau$ -decomposition for TDS with delay-dependent coefficients

Participants: Chi Jin [L2S], Keqin Gu [Illinois State University], Islam Boussaada, Silviu-Iulian Niculescu.

The standard frequency domain approaches for Time-delay systems analysis do not apply when the coefficients of the system are delay-dependent. Given a system with delay-dependent coefficients as well as a delay interval of interest, a method is proposed to find all the delay subintervals guaranteeing the asymptotic stability of the trivial solution. The crossing direction criteria is proposed which can be clearly interpreted from a geometrical two-parameter perspective [36], [52].

## 7.4. State and Output-feedback control design for (possibly fractional) time-delay systems

Participants: Catherine Bonnet, Caetano Cardeliquio, André Fioravanti [FEM-UNICAMP, Brazil].

We obtained this year new results for  $H_{\infty}$ -control synthesis via output-feedback through a finite order LTI system, called comparison system [42].

We also generalised those results for fractional systems.

The fractional comparison system was obtained and through LMIs we were able to calculate the  $H_{\infty}$ -norm for the fractional system and design a state-feedback control through the comparison system approach.

## 7.5. Stability and Stabilisability Through Envelopes for Retarded and Neutral Time-Delay Systems

**Participants:** Catherine Bonnet, Caetano Cardeliquio, Silviu Niculescu, André Fioravanti [FEM-UNICAMP, Brazil].

We presented a new approach to develop an envelope that engulfs all poles of a time-delay system.

Through LMIs we determined envelopes for retarded and neutral time-delay systems.

The envelopes proposed were not only tighter than the ones in the literature but they can also be applied to verify the stability of the system.

The approach was also used to design state-feedback controllers which cope with design requirements regarding  $\alpha - stability$ .

## 7.6. Backstepping with artificial delays

**Participants:** Frederic Mazenc, Michael Malisoff [LSU, USA], Laurent Burlion [ONERA], Victor Gibert [Airbus], Jerome Weston [LSU, USA].

We worked on the problem of improving a fundamental control design technique called backstepping.

We provided in [54] a new backstepping control design for time-varying systems with input delays. The result was obtained by the introduction of a constant 'artificial' pointwise delay in the input and a dynamic extension. Thus it is significantly different from backstepping results for systems with delay in the input as presented in previous contributions. The result in [54] ensures global asymptotic convergence for a broad class of partially linear systems with an arbitrarily large number of integrators. We used only one artificial delay, and we assumed that the nonlinear subsystems satisfy a converging-input-converging-state assumption. When the nonlinear subsystem is control affine with the state of the first integrator as the control, we provided sufficient conditions for our converging-input- converging-state assumption to hold.

# 7.7. Stability of time-varying systems with delay and Switched Nonlinear Systems

**Participants:** Frederic Mazenc, Hitay Ozbay [Blikent University, Turkey], Saeed Ahmed [Blikent University, Turkey], Silviu Niculescu, Michael Malisoff [LSU, USA].

Switched systems is a family of systems which is frequently encountered in practice and can be used to approximate time-varying systems to ease their stability analysis or control. In the two works [20] and [17], we provided results that are useful when it comes to analyze the stability of time-varying or switched systems with delay. In [20] we provided several significant applications of the trajectory approach developed recently by Mazenc and Malisoff. In two results, we used a Lyapunov function for a corresponding undelayed system to provide a new method for proving stability of linear continuous-time time-varying systems with bounded time-varying delays. Our main results used upper bounds on an integral average involving the delay. We also provided a novel reduction model approach that ensures global exponential stabilization of linear systems with a time-varying pointwise delay in the input, which allows the delay to be discontinuous and uncertain.

Three of our other works are devoted to switched systems. In [55] and [21], a new technique is proposed to ensure global asymptotic stability for nonlinear switched time-varying systems with time-varying discontinuous delays. It uses an adaptation of Halanay's inequality to switched systems and the trajectory based technique mentioned above. The result is applied to a family of linear time-varying systems with time-varying delays. In [53], we presented an extension of the trajectory based approach mentioned above for state feedback stabilization of switched linear continuous-time systems with a time-varying input delay. In contrast with finding classical common Lyapunov function or multiple Lyapunov functions for establishing the stability of the closed-loop switched system, the new trajectory based approach relies on verifying certain inequalities along the solution of a supplementary system. This study does not make any assumption regarding the stabilizability of all of the constituent modes of the switched system. Moreover, no assumption is needed about the differentiability of the delay and no constraint is imposed on the upper bound of the delay derivative.

In [17], we proved extensions of the celebrate Razumikhin's theorem for a general family of time-varying continuous and discrete-time nonlinear systems. Our results include a novel "strictification" technique for converting a nonstrict Lyapunov function into a strict one. We also provided new constructions of Lyapunov-Krasovskii functionals that can be used to prove robustness to perturbations. Our examples include a key model from identification theory, and they show how our method can sometimes allow broader classes of delays than the results in the literature.

## 7.8. Systems with Long Delays

**Participants:** Frederic Mazenc, Silviu Niculescu, Michael Malisoff [LSU,USA], Jerome Weston [LSU,USA], Ali Zemouche, Bin Zhou [Harbin Institute of Technology], Qingsong Liu [Harbin Institute of Technology].

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.

In [35], we studied the stabilization of linear systems with both state and input delays where the input delay can be arbitrarily large but exactly known. Observer-predictor based controllers are designed to predict the future states so that the input delay can be properly compensated. Necessary and sufficient conditions guaranteeing the stability of the closed-loop system are provided in terms of the stability of some simple linear time-delay systems refereed to as observer-error systems. Moreover, linear matrix inequalities are used to design both the state feedback gains and observer gains. Finally, a numerical example illustrates that the proposed approaches are more effective and safe to implement than the existing methods.

In [57], for a particular family of systems, we constructed observers in the case where the measured variables are affected by the presence of a point-wise time-varying delay. The key feature of the proposed observers is that the size of their gains is proportional to the inverse of the largest value taken by the delay. The main result is first presented in the case of linear chain of integrators and next is extended to nonlinear systems with specific nonlinearities (systems of feedforward form).

Two of our works are devoted to the development of the prediction technique based on sequential predictors. Let us recall that one of the key advantages of this method is that it circumvents the problem of constructing and estimating distributed terms in the control laws: instead of using distributed terms, our approach to handling longer delays is to increase the number of predictors. In [61], we provided a significant generalization of our previous results to cases with arbitrarily large feedback delay bounds, and where, in addition, current values of the plant state are not available to use in the sequential predictors. We illustrate our work in a pendulum example. In [18], we provided a new sequential predictors approach for the exponential stabilization of linear time-varying systems. Our method allows arbitrarily large input delay bounds, pointwise time-varying input delays and uncertainties. We obtain explicit formulas to find lower bounds for the number of required predictors.

## 7.9. Nonlinear Observer Design via LMIs

**Participants:** Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Hieu Trinh [Deakin University, Australia], Yan Wang [University of Minneapolis, USA], Michel Zasadzinski [CRAN], Hugues Rafaralahy [CRAN], Boulaid Boulkroune [Flanders Make, Lommel, Belgium], Gridsada Phanomchoeng [Chulalongkorn University, Thailand], Khadidja Chaib-Draa [University of Luxembourg], Mohamed Darouach [CRAN], Marouane Alma [CRAN], Holger Voos [University of Luxembourg].

• Observer Design for Lipschitz and Monotonic nonlinear systems using LMIs:

New LMI (Linear Matrix Inequality) design techniques have been developed to address the problem of designing performant observers for a class of nonlinear systems. The developed techniques apply to both locally Lipschitz as well as monotonic nonlinear systems, and allows for nonlinear functions in both the process dynamics and output equations [59], [34]. The LMI design conditions obtained are less conservative than all previous results proposed in literature for these classes of nonlinear systems. By judicious use of 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. Although this application was the main motivation of this work, the proposed techniques have been applied to an anaerobic digestion model for different contexts [43], [44], [45].

HG/LMI Observer:

A new high-gain observer design method with lower gain compared to the standard high-gain observer was proposed [62]. 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 that we can call "smart high-gain observer". The aim of this research is the application of this new observer design to estimate some variables in vehicle applications and other real-world applications.

• Dual Spatially Separated Sensors for Enhanced Estimation:

Inspired by the function of spatially separated sensory organs found in nature, we explored the use of dual spatially separated sensors for enhanced estimation in modern engineering applications [26]. To illustrate the interest of dual spatially separated sensors, some real applications have been considered: 1) Adaptive parameter and state estimation in magnetic sensors; 2) Estimation of an unknown disturbance input in an automotive suspension; 3) Separation of inputs based on their direction of action in a digital stethoscope. Both analytical observer design developments and experimental evaluation of the results have been provided.

### 7.10. Observer-Based Stabilization of Uncertain Nonlinear Systems

**Participants:** Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Yan Wang [University of Minneapolis, USA], Fazia Bedouhne [University of Tizi-Ouzou, Algeria], Hamza Bibi [University of Tizi-Ouzou, Algeria], Abdel Aitouche [CRIStAL, Lille].

• Relaxed LMI conditions for switched systems and LPV systems:

By exploiting the Finsler's lemma in a non-standard way, we derived new LMI conditions. This technique has been applied to linear switched systems with uncertain parameters [10], [40] and LPV (Linear Parameter Varying) systems with inexact parameters [39], respectively. In each case, the Finsler's inequality is exploited in a convenient way to get additional decision variables which render the LMIs less conservative than those existing in the literature. In addition to analytical comparisons, several numerical examples have been used to show the superiority of the proposed new LMI conditions.

• From LMI relaxations to sequential LMI algorithm:

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 [28]. 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. In the application part, a vehicle lateral control problem is presented to demonstrate the applicability of the proposed algorithm to a real-world estimated state feedback control design.

# 7.11. Analysis of PWA control of discrete-time linear dynamics in the presence of variable input delay

Participants: Sorin Olaru, Mohammed Laraba [CentraleSupélec], Silviu Niculescu.

We have addressed the robustness of a specific class of control laws, namely the piecewise affine (PWA) controllers, defined over a bounded region of the state-space. More precisely, we were interested in closed-loop systems emerging from linear dynamical systems controlled via feedback channels in the presence of varying transmission delays by a PWA controller defined over a polyhedral partition of the state-space. We exploit the fact that the variable delays are inducing some particular model uncertainty. Our objective was to characterize the delay invariance margins: the collection of all possible values of the time-varying delays for which the positive invariance of the corresponding region is guaranteed with respect to the closed-loop dynamics. These developments are proving to be useful for the analysis of different design methodologies and, in particular, for model predictive control (MPC) approaches. The proposed delay margin describes the admissible transmission delays for an MPC implementation. From a different perspective, the delay margin further characterizes the fragility of an embedded MPC implementation via the on-line optimization and subject to variable computational time.

# 7.12. On the precision in polyhedral partition representation and the fragility of PWA control

Participants: Sorin Olaru, Rajesh Koduri [CentraleSupélec], Pedro Rodriguez [CentraleSupélec].

Explicit model predictive control (EMPC) solves a multi-parametric Quadratic Programming (mp-QP) problem for a class of discrete-time linear system with linear inequality constraints. The solution of the EMPC problem in general is a piecewise affine control function defined over non-overlapping convex polyhedral regions composing a polyhedral partition of the feasible region. In this work, we considered the problem of perturbations on the representation of the vertices of the polyhedral partition. Such perturbations may affect some of the structural characteristics of the PWA controller such as *non-overlapping within the regions* or *the closed-loop invariance*. We first showed how a perturbation affects the polyhedral regions and evoked the overlapping within the modified polyhedral regions. The major contribution of this work is to analyze to what extend the non-overlapping and the invariance characteristics of the PWA controller can be preserved when the perturbation takes place on the vertex representation. We determined a set called sensitivity margin to characterize for admissible perturbation preserving the non-overlapping and the invariance property of the controller. Finally, we show how to perturb multiple vertices sequentially and reconfigure the entire polyhedral partition

## 7.13. Convex Lifting: Theory and Control Applications

**Participants:** Sorin Olaru, Martin Gulan [STU, Bratislava, Slovaquie], Ngoc Anh Nguyen [J. Kepler Univ., Linz, Austria], Pedro Rodriguez [CentraleSupélec].

We introduced the *convex lifting* concept which was proven to enable significant implementation benefits for the class of piecewise affine controllers. Accordingly, two different algorithms to construct a convex lifting for a given polyhedral/polytopic partition were presented. These two algorithms rely on either the vertex or the halfspace representation of the related polyhedra. Also, we introduced an algorithm to refine a polyhedral partition, which does not admit a convex lifting, into a convexly liftable one. Furthermore, two different schemes are put forward to considerably reduce both the memory footprint and the runtime complexity which play a key role in implementation of piecewise affine controllers. These results have been illustrated via a numerical example and a complexity analysis.

## 7.14. Attitude control

Participants: Frederic Mazenc, Maruthi Akella [Univ. of Texas, USA], Sungpil Yang [Univ. of Texas, USA].

In [31], we addressed adaptive control of specific Euler-Lagrange systems: rigid-body attitude control, and the n-link robot manipulator. For each problem, the model parameters are unknown but the lower bound of the smallest eigenvalue of the inertia matrix is assumed to be known. The dynamic scaling Immersion and Invariance (I&I) adaptive controller is proposed to stabilize the system without employing a filter for the regressor matrix. A scalar scaling factor is instead implemented to overcome the integrability obstacle that arises in I&I adaptive control design. First, a filter-free controller is proposed for the attitude problem such that the rate feedback gain is proportional to the square of the scaling factor in the tracking error dynamics. The gain is then shown to be bounded through state feedback while achieving stabilization of the tracking error. The dynamic scaling factor increases monotonically by design and may end up at a finite but arbitrarily large value. However, by introducing three more dynamic equations, the non-decreasing scaling factor can be removed from the closed-loop system. Moreover, the behavior of dynamic gain is dictated by design parameters so that its upper bound is limited by a known quantity and its final value approaches the initial value. A similar approach for the dynamic gain design is also applied to a filter-dependent controller where a filter for the angular rate is utilized to build a parameter estimator. Unlike the filter-free design, the filterdependent controller admits a constant gain for the rate feedback while the dynamic scaling factor rather appears in the filter. Finally, the proposed design is applied to robot manipulator systems. Spacecraft attitude and 2-link planar robot tracking problems are considered to demonstrate the performance of the controllers through simulations.

The work [32] builds on the preliminary results by generalizing to the tracking case and some further analysis of the filter-free case. Extending the strictification technique, a partially strict Lyapunov function is constructed toward establishment of stability and ultimate boundedness properties for the closed-loop system. With known upper bounds of the magnitude of measurement errors, disturbance torques, and parameter uncertainties, a feasible range for the feedback gains is derived in terms of bounds on the initial conditions in such a way to ensure asymptotic convergence of all closed-loop signals to within a residual set. In spite of the nonlinear structure of the kinematics and dynamics of the problem, however, the closed-loop system is rigorously analyzed through the standard Lyapunov analysis methods. This is achieved owing to the fact that the strictified Lyapunov function allows us to deal with this nontrivial problem in a standard way. As the passivity-based controller is not new for the attitude control problem, the key contribution of this paper is a theoretical analysis of the ideal case design in the presence of uncertainties through Lyapunov stability analysis.

## 7.15. Active Vibration Control of thin structures

**Participants:** Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S], Hakki Unal [Anadolu University], Toma Vyhlidal [Czech Technical University].

The problem of active vibrations damping of thin mechanical structures is a topic that has received great attention by the control community for several years, especially, when actuators and sensors are based on piezoelectric materials. For mechanical structures that are deformable, piezoelectric materials are used as strain sensors or strain actuators. With an appropriate controller, they allow to achieve shape control or the active damping of multi-modal vibrations thanks to their very large bandwidth. In this area, the major challenge is the design of controllers able to damp the most vibrating modes in a specified low-frequency bandwidth while ensuring robustness against high-frequency modes, outside the bandwidth of interest, often unmodelled or weakly modelled. The inherent feature of this kind of systems is that they arise robustness issues when they are tackled with finite dimensional control tools. A delayed state-feedback control strategies based on rightmost spectral values assignment allowing a fast vibration damping are proposed in [69], [41], [11].

## 7.16. Automatic Train Supervision for a CBTC Suburban Railway Line Using Multiobjective Optimization

Participants: Guillaume Sandou, Juliette Pochet [SNCF], Sylvain Baro [SNCF].

Communication-based train control (CBTC) systems have been deployed on subway lines to increase capacities on existing infrastructures. For the same purpose, CBTC systems are to be deployed on suburban railway lines where operating principles and constraints are significantly different. A regulation method for CBTC trains on a suburban line has been developed. This method is designed to combine CBTC functionalities with suburban operating principles. It includes a traffic management method in station, and a rescheduling method in case of disturbances. The proposed regulation method is integrated into the railway system simulation tool SIMONE developed by SNCF. This simulation tool includes models of the whole CBTC system, as well as the classic signaling system, train dynamics and railway infrastructures. Models of these different agents are described. The integration of the proposed regulation method into the tool SIMONE allows evaluating performances while taking into account the functional complexity of a CBTC railway system. The approach is illustrated with a realistic case: simulations of a CBTC traffic on the urban part of a railway line in the Paris region network are described. The proposed regulation method shows interesting results in disturbed situations according to the railway operating principles [60].

## 7.17. A Distributed Consensus Control Under Disturbances for Wind Farm Power Maximization

**Participants:** Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [CentraleSupélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

We have addressed the problem of power sharing among the wind turbines (WTs) belonging to a wind farm. The objective is to maximize the power extraction under the wake effect, and in the presence of wind disturbances. Because of the latter, WTs may fail in respecting the optimal power sharing gains. These are restored by employing a consensus control among the WTs. In particular, under the assumption of discrete-time communication among the WTs, we propose a distributed PID-like consensus approach that enhances the rejection of the wind disturbances by providing the power references to the local WT controllers. The latter are designed by employing a novel feedback linearization control that, acting simultaneously on the WT rotor speed and the pitch angle, guarantees the tracking of general deloaded power references. The obtained results are validated on a 6-WT wind farm example. [50].

## 7.18. Distributed Particle Swarm Optimization Algorithm for the Optimal Power Flow Problem

**Participants:** Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [CentraleSupélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

The distributed optimal power flow problem has been addressed. No assumptions on the problem cost function, and network topology are needed to solve the optimization problem. A particle swarm optimization algorithm is proposed, based on Deb's rule to handle hard constraints. Moreover, the approach enables to treat a class of distributed optimization problems, via a population based algorithm, in which the agents share a common optimization variable. A simulation example is provided, based on a 5-bus electric grid. [51].

## 7.19. Chemostat

Participants: Frederic Mazenc, Michael Malisoff [LSU,USA], Gonzalo Robledo [Univ. de Chile, Chile].

A chemostat is a fundamental bioreactor used to study the behavior of microorganisms. Many different types of chemostats exist, and many different types of models represent them.

We studied in [56] a chemostat model with an arbitrary number of competing species, one substrate, and constant dilution rates. We allowed delays in the growth rates and additive uncertainties. Using constant inputs of certain species, we derived bounds on the sizes of the delays that ensure asymptotic stability of an equilibrium when the uncertainties are zero, which can allow persistence of multiple species. Under delays and uncertainties, we provided bounds on the delays and on the uncertainties that ensure a robustness property of input-to-state stability with respect to uncertainties.

In [16], we provided a new control design for chemostats, under constant substrate input concentrations, using piecewise constant delayed measurements of the substrate concentration. Our growth functions can be uncertain and are not necessarily monotone. The dilution rate is the control. We use 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.

## 7.20. Qualitative/quantitative analysis of a delayed chemical model

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Hakki Unal [Anadolu University].

The Belousov-Zhabotinsky reaction is a complex chemical reaction exhibiting sustained oscillations observed in some real biological oscillators. However, its oscillatory behavior is represented by a simple mechanism, called the Oregonator. A qualitative/quantitative analysis of a two-delay Oregonator based chemical oscillator is considered where the delay effect in dynamics is investigated; the existence of positive equilibrium point, the stability and boundedness of solutions for positive initial conditions are explored [27].

## 7.21. Mathematical Modelling of Acute Myeloid Leukemia

**Participants:** Catherine Bonnet, Jean Clairambault [MAMBA project-team], François Delhommeau [IN-SERM 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, Hitay Özbay [Bilkent University].

The ALMA3-project is about the modeling and analysis of healthy and unhealthy cell population dynamics, with a particular focus on hematopoiesis, which is the process of blood cell production and continuous replenishment. We point out that medical research is now looking for new combined targeted therapies able to overcome the challenge of cancer cells (e.g. to stop overproliferation, to restore normal apoptosis rates and differentiation of immature cells, and to avoid the high toxicity effects that characterize heavy non-selective chemotherapy). In that quest, the ultimate goal behind mathematical studies is to provide some inputs that should help biologists to suggest and test new treatment, and to contribute within multi-disciplinary groups in the opening of new perspectives against cancer. Thus, our research project is imbued within a similar spirit and fits the expectations of a better understanding of the behavior of healthy and unhealthy blood cell dynamics. It involve intensive collaboration with hematologists from Saint Antoine hospital in Paris, and aims to analyze the cell fate evolution in treated or untreated leukemia, allowing for the suggestion of new anti-leukemic combined chemotherapy.

In 2017, we have discussed some of the issues that are related to the modeling of the cell cycle, with particular insight into hematopoietic systems. For instance, i) we introduced and studied for the first time the effect of cell plasticity (dedifferentiation and transdifferentiation mechanisms) in the class of models that we focus on, and ii) we considered the effect of cell-arrest (i.e. some cells can be arrested during their cell-cycle) in models with several maturity stages. Stability features of the resulting biological models are highlighted, since systems trajectories reflect the most prominent healthy or unhealthy behaviors of the biological process under study. We indeed perform stability analysis of systems describing healthy and unhealthy situations, particularly in the case of acute myeloblastic leukemia (AML). More precisely, these are nonlinear timedelay systems that involve finite or infinite distributed delay terms, with possibly time-varying parameters. We pursue the objectives of earlier works in order to understand the interactions between the various parameters and functions involved in the mechanisms we study. Sometimes, we extend the stability analysis and the application of some already existing models, whereas news models and variants are other times introduced to cover novel biological evidences, such as: mutations accumulation and cohabitation between ordinary and mutated cells in niches, control and eradication of cancer stem cells, cancer dormancy and cell plasticity. In fact, 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. So, this year, we have progressed on our project and we have extended our works in order to develop the modeling and analysis aspects in cancer dormancy by including the effects of immuno-therapies in AML [48]. Lyapunovlike techniques have been used in this work in order to derive global or local exponential stability conditions for that class of differential-difference systems. Finally, in [49], we have modeled the role played by growth factors -these are hormone-like molecules- or drugs on the regulation of various biological features that are involved in hematopoiesis.

## 7.22. Analysis of Dengue Fever SIR Model with time-varying parameters

**Participants:** Stefanella Boatto [Univ Feder Rio de Janeiro], Catherine Bonnet, Frédéric Mazenc, Le Ha Vy Nguyen.

Dengue fever is an infectious viral disease occurring 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 worldwide. We continued this year our study on modeling of dengue epidemics.

We have first considered a SIR model with birth and death terms and time-varying infectivity parameter  $\beta(t)$ . In the particular case of a sinusoidal parameter, we showed that the average Basic Reproduction Number  $R_o$ , introduced in [Bacaër & Guernaoui, 2006], is not the only relevant parameter and we emphasized the rôle played by the initial phase, the amplitude and the period. For a (general) periodic infectivity parameter  $\beta(t)$  a periodic orbit exists, as already proved in [Katriel, 2014]. In the case of a slowly varying  $\beta(t)$  an approximation of such a solution is given, which is shown to be asymptotically stable under an extra assumption on the slowness of  $\beta(t)$ . For a non necessarily periodic  $\beta(t)$ , all the trajectories of the system are proved to be attracted into a tubular region around a suitable curve, which is then an approximation of the underlying attractor. Numerical simulations are given [68].

In other to study the effects of urban human mobility on Dengue epidemics, we have considered a SIR-network model (still with birth and death rates). The same model without these rates was introduced in [72].

In the case of constant infection rates, we first examine networks of two nodes. For arbitrary network topologies, some general properties of the equilibrium points are obtained. Then for several specific topologies, we derive explicit expressions of multiple equilibrium points and characterize their stability properties. We extend the study to networks with an arbitrary number of nodes and obtain sufficient conditions for global asymptotic stability of the disease-free equilibrium point.

In the case of time-varying infection rates and networks of arbitrary number of nodes, we introduce a specific topology which leads to a simplification of the network: the dynamics of the total population is described by the classical SIR model. This fact, together with the results of the team on the SIR model, allows a complete characterization of the stability properties of the system, especially the approximation of the epidemic attractor.

## **GECO Project-Team**

## 7. New Results

## 7.1. New results

Let us list some the new results in sub-Riemannian geometry and hypoelliptic diffusion obtained by GECO's members.

- On a sub-Riemannian manifold we define two type of Laplacians. The macroscopic Laplacian Δ<sub>ω</sub>, as the divergence of the horizontal gradient, once a volume ω is fixed, and the microscopic Laplacian, as the operator associated with a geodesic random walk. In [1] we consider a general class of random walks, where all sub-Riemannian geodesics are taken in account. This operator depends only on the choice of a complement c to the sub-Riemannian distribution, and is denoted L<sub>c</sub>. We address the problem of equivalence of the two operators. This problem is interesting since, on equiregular sub-Riemannian manifolds, there is always an intrinsic volume (e.g. Popp's one P) but not a canonical choice of complement. The result depends heavily on the type of structure under investigation:
  - On contact structures, for every volume  $\omega$ , there exists a unique complement c such that  $\Delta_{\omega} = L_c$ .
  - On Carnot groups, if H is the Haar volume, then there always exists a complement c such that  $\Delta_H = L_c$ . However this complement is not unique in general.
  - For quasi-contact structures, in general,  $\Delta_P = L_c$  for any choice of c. In particular,  $L_c$  is not symmetric w.r.t. Popp's measure. This is surprising especially in dimension 4 where, in a suitable sense,  $\Delta_P$  is the unique intrinsic macroscopic Laplacian.

A crucial notion that we introduce here is the N-intrinsic volume, i.e. a volume that depends only on the set of parameters of the nilpotent approximation. When the nilpotent approximation does not depend on the point, a N-intrinsic volume is unique up to a scaling by a constant and the corresponding N-intrinsic sub-Laplacian is unique. This is what happens for dimension smaller or equal than 4, and in particular in the 4-dimensional quasi-contact structure mentioned above.

- In sub-Riemannian geometry the coefficients of the Jacobi equation define curvature-like invariants. We show in [4] that these coefficients can be interpreted as the curvature of a canonical Ehresmann connection associated to the metric, first introduced by Zelenko and Li. We show why this connection is naturally nonlinear, and we discuss some of its properties.
- In [6] we study the cut locus of the free, step two Carnot groups G<sub>k</sub> 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 by O. Myasnichenko, by exhibiting sets of cut points C<sub>k</sub> ⊂ G<sub>k</sub> which, for k ≥ 4, are strictly larger than conjectured ones. While the latter were, respectively, smooth semi-algebraic sets of codimension Θ(k<sup>2</sup>) and semi-algebraic sets of codimension Θ(k), the sets C<sub>k</sub> are semi-algebraic and have codimension 2, yielding the best possible lower bound valid for all k on the size of the cut locus of G<sub>k</sub>. Furthermore, we study the relation of the cut locus with the so-called abnormal set. 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<sub>k</sub>. The question whether C<sub>k</sub> coincides with the cut locus for k ≥ 4 remains open.

New results on complex systems with hybrid or switched components are the following.

• In [2] we address the exponential stability of a system of transport equations with intermittent damping on a network of  $N \ge 2$  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 an explicit formula for the solutions of this system, which allows one to track down the effects of the intermittent damping.

• In [3] we study the relative controllability of linear difference equations with multiple delays in the state by using a suitable formula for the solutions of such systems in terms of their initial conditions, their control inputs, and some matrix-valued coefficients obtained recursively from the matrices defining the system. 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, in a sense that we make precise. Finally, we provide an upper bound on the minimal controllability time for a system depending only on its dimension and on its largest delay.

Finally, a new contribution has been proposed in the domain of the control of quantum systems. More precisely, in [5] we consider the bilinear Schrödinger equation with discrete-spectrum drift. We show, for  $n \in \mathbb{N}$  arbitrary, exact controllability in projections on the first n given eigenstates. The controllability result relies on a generic controllability hypothesis on some associated finite-dimensional approximations. The method is based on Lie-algebraic control techniques applied to the finite-dimensional approximations coupled with classical topological arguments issuing from degree theory.

## **I4S Project-Team**

## 7. New Results

## 7.1. Outdoor InfraRed Thermography

## 7.1.1. Joint thermal and electromagnetic diagnostics

Participants: Nicolas Le Touz, Jean Dumoulin.

In this study, we present an inversion approach to detect and localize inclusions in thick walls under natural solicitations. The approach is based on a preliminary analysis of surface temperature field evolution with time (for instance acquired by infrared thermography); subsequently, this analysis is improved by taking advantage of a priori information provided by ground penetrating radar reconstruction of the structure under investigation. In this way, it is possible to improve the accuracy of the images achievable with the standalone thermal reconstruction method in the case of quasiperiodic natural excitation. [19]

## 7.1.2. Long term monitoring of transport infrastructures: from deployment to standardization Participants: Antoine Crinière, Jean Dumoulin, Laurent Mevel.

Long term monitoring of transport infrastructures by infrared thermography has been studied and tested on different structures. A first standalone infrared system architecture developed is presented and discussed. Results obtained with such system on different Civil Engineering structures are presented. Some data processing approaches and inverse thermal model for data analysis are introduced and discussed. Lessons learned from experiments carried out in outdoor with such system are listed and analyzed. Then, a new generation of infrared system architecture is proposed. Finally, conclusions and perspectives are addressed.[29], [46]

## 7.1.3. Infrared data reconstruction and calibration for long term monitoring

Participants: Thibaud Toullier, Jean Dumoulin, Laurent Mevel.

This study focuses on the evaluation and improvement of thermal instrumentation solutions for long-term monitoring of next-generation transport infrastructure. A test site was equipped with thermocouples and an infrared thermography system coupled with monitoring of environmental parameters. A method of spatial reconstruction of infrared images is presented. Measurement data acquired on site and then post-processed are analysed over time. A conclusion on the results achieved and prospects are proposed [48]

## 7.2. Data management of Smart territories and cities

Participants: Antoine Crinière, Jean Dumoulin.

Highly instrumented Smart-cities, which are now a common urban policies, are facing problems of management and storage of a large volume of data coming from an increasing number of sources. This study presents a data compression method by predictive coding of spatially correlated multi-source data based on reference selection and prediction by Kriging [47]

## 7.3. Smarts roads and R5G

**7.3.1.** Energy exchange modelization and infrared monitoring for hybrid pavement structure **Participants:** Nicolas Le Touz, Thibaud Toullier, Jean Dumoulin.

In those studies, we evaluate by numerical modelling the energy inputs that could occur in a hybrid pavement structure with a semi-transparent or opaque wearing course bonded to a porous base layer, the seat of a heat transfer fluid circulation. The digital studies conducted propose a coupled resolution of various thermal phenomena: diffusion/convection in the case of an opaque surface drainage pavement, and diffusion/convection/radiation for a pavement with a semi-transparent surface. Coupled equation systems are solved numerically using the finite element method. This model was developed directly on a Matlab kernel. In a second time, laboratory experiments on small specimen were carried out and the surface temperature was monitored by infrared thermography. Results obtained are analyzed and performances of the numerical model for real scale outdoor application are discussed .[35], [34]

#### 7.3.2. Phase change materials characterization

### Participant: Jean Dumoulin.

In a costs reduction and comfort requirements context, the use of phase change materials (PCM) is a sustainable and economical answer. For transportation infrastructures and winter maintenance, they avoid ice occurrence or snow accumulation. Their characteristics, and more specifically, the solid to liquid phase transition temperature and enthalpy, are usually obtained through DSC. Raman spectroscopy can bring answers and information on their microstructures. The liquid to solid phase change was investigated on three PCM, a paraffin, formic acid and diluted formic acid. A comparison made on freezing temperature obtained through DSC, Raman spectroscopy associated with chemiometrics indicated a consistency between the methods. Raman spectroscopy coupled with multivariate data analysis allowed the identification of an additional specificity in the freezing process of the paraffin. All methods provided results consistent between each other, although some differences between literature and experimental freezing temperatures of the considered PCM were observed in all cases. [20], [53]

## 7.4. Methods for building performance assessment

## 7.4.1. Building performance assessment

Participants: Jordan Brouns, Alexandre Nassiopoulos.

Two additive thermal sources are generally not simultaneously distinguishable from the only observation of their effect on the heat balance. However, there are cases where information about the variation regularity of these sources is known. This is typically the case of convective internal gains in the building, for which the use scenarios create discontinuous inputs while heat gains relating to the air leakage are regular in time. In the present paper, we introduce a method aiming to distinguish heat sources using this a priori knowledge about their dynamics. We provide numerical and experimental evidence that the method succeeds in separating/distinguishing these kind of sources. This method could be applied to the identification of the occupancy rate for measurement and verification plans or smart home systems such as learning thermostats. [16]

## 7.5. System identification

## 7.5.1. Variance estimation of modal parameters from subspace-based system identification Participants: Michael Doehler, Laurent Mevel.

This work has been carried out in collaboration with Palle Andersen.

Subspace-based system identification allows the accurate estimation of the modal parameters (natural frequencies, damping ratios, mode shapes) from output-only measurements, amongst others with data-driven methods like the Unweighted Principal Component (UPC) algorithm. Due to unknown excitation, measurement noise and finite measurements, all modal parameter estimates are inherently afflicted by uncertainty. The information on their uncertainty is most relevant to assess the quality of the modal parameter estimates, or when comparing modal parameters from different datasets. A method for variance estimation is presented for the variance computation of modal parameters for the UPC subspace algorithm. Developing the sensitivities of the modal parameters with respect to the output covariances, the uncertainty is propagated from the measurements to the modal parameters from UPC. The resulting variance expressions are easy to evaluate and computationally tractable when using an efficient implementation. In a second step, the uncertainty information of the stabilization diagram is used to extract appropriately weighted global mode estimates and their variance. The method is applied to experimental data from the Z24 Bridge [30].

## 7.5.2. Bayesian parameter estimation for parameter varying systems using interacting Kalman filters

Participants: Antoine Crinière, Laurent Mevel, Jean Dumoulin, Subhamoy Sen.

This work is in collaboration with F. Cerou of ASPI team at Inria.

Standard filtering techniques for structural parameter estimation assume that the input force either is known exactly or can be replicated using a known white Gaussian model. Unfortunately for structures subjected to seismic excitation, the input time history is unknown and also no previously known representative model is available. A novel algorithm is proposed to estimate the force as additional state in parallel to the system parameters. Two concurrent filters are employed for parameters and force respectively, mixing interacting Particle Kalman filter and another filter employed to estimate the seismic force acting on the structure [38], [49].

#### 7.5.3. From structurally independent local LTI models to LPV model

Participant: Qinghua Zhang.

This work on linear parameter varying (LPV) system identification has been carried out in collaboration with Lennart Ljung (Linköping University, Sweden).

The local approach to LPV system identification consists in interpolating individually estimated local linear time invariant (LTI) models corresponding to fixed values of the scheduling variable. It is shown in this work that, without any global structural assumption of the considered LPV system, individually estimated local state-space LTI models do not contain sufficient information for determining similarity transformations making them coherent. Nevertheless, it is possible to estimate these similarity transformations from input-output data under appropriate excitation conditions [21].

## 7.5.4. Stability of the Kalman filter for output error systems

#### Participant: Qinghua Zhang.

The stability of the Kalman filter is classically ensured by the uniform complete controllability regarding the process noise and the uniform complete observability of linear time varying systems. Recently we have studied the stability of the Kalman filter for output error (OE) systems, in which the process noise is totally absent. In this case the classical stability analysis assuming the controllability regarding the process noise is thus not applicable. Our first efforts were focused on continuous time systems, whereas discrete time systems have been studied since last year. It is shown in this work that the uniform complete observability is sufficient to ensure the stability of the Kalman filter applied to time varying OE systems, regardless of the stability of the OE systems [22].

#### 7.5.5. Reduced-order interval-observer design for dynamic systems with time-invariant uncertainty

Participant: Qinghua Zhang.

This work on interval-based state estimation has been carried out in collaboration with Vicenç Puig's team (Universitat Politècnica de Catalunya, Spain). The reported work addresses in particular the design of reducedorder interval-observers for dynamic systems with both time-invariant and time varying uncertainties. Because of the limitations of the set-based approach and the wrapping effect to deal with interval-observers, the trajectory-based interval-observer approach is used with an appropriate observer gain. Due to difficulties to satisfy the conditions for selecting a suitable gain to guarantee the positivity of the resulting observer, a reduced-order observer is designed to increase the degree of freedom when selecting the observer gain and to reduce the computational complexity. Simulation examples illustrates the effectiveness of the proposed approach [37].

# 7.5.6. 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).

Recently, a subspace fitting approach has been proposed for vibration-based finite element model updating. The approach makes use of subspace-based system identification, where the extended observability matrix is estimated from vibration measurements. Finite element model updating is performed by correlating the model-based observability matrix with the estimated one. However, estimates from vibration measurements are inherently exposed to uncertainty. A covariance estimation procedure for the updated model parameters is proposed, which propagates the data-related covariance to the updated model 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. Simulated vibration signals and experimental data of a beam validate the method [18].

## 7.6. Damage diagnosis

#### 7.6.1. Damage detection by perturbation analysis and additive change detection theory

Participants: Michael Doehler, Laurent Mevel, Qinghua Zhang.

The monitoring of mechanical systems aims at detecting damages at an early stage, in general by using output-only vibration measurements under ambient excitation. In this paper, a method is proposed for the detection and isolation of small changes in the physical parameters of a linear mechanical system. Based on a recent work where the multiplicative change detection problem is transformed to an additive one by means of perturbation analysis, changes in the eigenvalues and eigenvectors of the mechanical system are considered in the first step. In a second step, these changes are related to physical parameters of the mechanical system. Finally, another transformation further simplifies the detection and isolation problem into the framework of a linear regression subject to additive white Gaussian noises, leading to a numerically efficient solution of the considered problems. A numerical example of a simulated mechanical structure is reported for damage detection and localization [31].

## 7.6.2. Damage localization using the statistical subspace damage localization method

Participants: Michael Doehler, Laurent Mevel, Saeid Allahdadian.

This work is happening during a thesis in collaboration with C. Ventura at UBC, Vancouver.

In this paper the statistical subspace damage localization (SSDL) method is employed in localizing the damage in a real structure, namely the Yellow frame. The SSDL method is developed for real testing conditions and tested in two damage configurations. It was demonstrated that the SSDL method can localize the damage robustly in the Yellow frame for simple and multiple distinct damage scenarios using the analytical modal parameters. The method is described and its effectiveness is demonstrated [24].
## 7.6.3. Stochastic Subspace-Based Damage Detection with Uncertainty in the Reference Null Space

Participants: Michael Doehler, Laurent Mevel, Eva Viefhues.

This work is happening during a thesis in collaboration with F. Hille at BAM, Berlin.

This paper deals with uncertainty considerations in damage diagnosis using the stochastic subspace-based damage detection technique. With this method, a model is estimated from data in a (healthy) reference state and confronted to measurement data from the possibly damaged state in a hypothesis test. Previously, only the uncertainty related to the measurement data was considered in this test, whereas the uncertainty in the estimation of the reference model has not been considered. We derive a new test framework, which takes into account both the uncertainties in the estimation of the reference model as well as the uncertainties related to the measurement data. Perturbation theory is applied to obtain the relevant covariances. In a numerical study the effect of the new computation is shown, when the reference model is estimated with different accuracies, and the performance of the hypothesis tests is evaluated for small damages. Using the derived covariance scheme increases the probability of detection when the reference model estimate is subject to high uncertainty, leading to a more reliable test [41].

#### 7.6.4. Statistical damage localization with stochastic load vectors

Participants: Md Delwar Hossain Bhuyan, Michael Doehler, Laurent Mevel, Guillaume Gautier.

This work is in collaboration with F. Schoefs and Y. Lecieux, GEM, Nantes.

The Stochastic Dynamic Damage Locating Vector (SDDLV) method is a damage localization method based on both a Finite Element (FE) model of the structure and modal parameters estimated from 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 from 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. An important theoretical limitation was that the number of modes used in the computation could not be higher than the number of sensors located on the structure. In this paper, the SDDLV method has been extended with a joint statistical approach for multiple mode sets, overcoming this restriction on the number of modes. Another problem is that the performance of the method can change considerably depending of the Laplace variable where the transfer function is evaluated. Particular attention is given to this choice and how to optimize it. The new approach is validated in numerical simulations and on experimental data. 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 [15], [52], [27].

#### 7.6.5. Transfer matrices-based statistical damage localization and quantification

Participants: Md Delwar Hossain Bhuyan, Michael Doehler, Laurent Mevel, Guillaume Gautier.

This work is in collaboration with GEM, Nantes and C. Ventura at UBC, Nantes.

Vibration measurements and a finite element model are used to locate loss of stiffness in a steel frame structure at the University of British Columbia. The Stochastic Dynamic Damage Locating Vector (SDDLV) is compared to a sensitivity based approach developed by the authors. Both approaches have in common to be built on the estimated transfer matrix difference between reference and damaged states. Both methods are tested for localization and quantification on a structure at University of British Columbia [26], [28].

## 7.6.6. Statistical damage localization based on Mahalanobis distance Participant: Michael Doehler.

This work is in collaboration with Aalborg University, Structural Vibration Solutions and Universal Foundation in Denmark during the thesis of S. Gres (Aalborg University).

In this paper, a new Mahalanobis distance-based damage detection method is studied and compared to the wellknown subspace-based damage detection algorithm. Methods are implemented using control charts to enhance the resolution of the damage detection. The damage indicators are evaluated based on the ambient vibration signals from numerical simulations on a novel offshore support structure and experimental example of a full scale bridge. The results reveal that the performance of the two damage detection methods is similar, hereby implying merit of the new Mahalanobis distance-based approach, as it is less computationally complex [32].

## 7.6.7. On the value of Information for SHM

Participant: Michael Doehler.

This work is issued from the COST Action TU1402.

The concept of value of information (VoI) enables quantification of the benefits provided by structural health monitoring (SHM) systems in principle. Its implementation is challenging, as it requires an explicit modelling of the structural system's life cycle, in particular of the decisions that are taken based on the SHM information. In this paper, we approach the VoI analysis through an influence diagram (ID), which supports the modelling process. We provide a simple example for illustration and discuss challenges associated with real-life implementation [39].

## 7.6.8. Structural system reliability and damage detection information

Participant: Michael Doehler.

This work is in collaboration with S. Thöns (DTU) during the thesis of L. Long (BAM).

This paper addresses the quantification of the value of damage detection system and algorithm information on the basis of Value of Information (VoI) analysis to enhance the benefit of damage detection information by providing the basis for its optimization before it is performed and implemented. The approach of the quantification the value of damage detection information builds upon the Bayesian decision theory facilitating the utilization of damage detection performance models, which describe the information and its precision on structural system level, facilitating actions to ensure the structural integrity and facilitating to describe the structural system performance and its functionality throughout the service life. The structural system performance is described with its functionality, its deterioration and its behavior under extreme loading. The structural system reliability given the damage detection information is determined utilizing Bayesian updating. The damage detection performance is described with the probability of indication for different component and system damage states taking into account type 1 and type 2 errors. The value of damage detection information is then calculated as the difference between the expected benefits and risks utilizing the damage detection information is determined, demonstrating Pratt truss system, the value of damage detection information is determined, demonstrating the potential of risk reduction and expected cost reduction [36].

## 7.6.9. Estimation of a cable resistance profile with readaptation of mismatched measurement instrument

#### Participants: Nassif Berrabah, Qinghua Zhang.

As the cumulative length of electric cables in modern systems is growing and as these systems age, it becomes of crucial importance to develop efficient tools to monitor the condition of wired connections. Therein, in contrast to hard faults (open or short circuits), the diagnosis of soft-faults requires a particular effort. Indeed, these faults are more difficult to detect, yet they are sometimes early warning signs of more important failures. In a previous paper, we proposed a method to compute the resistance profile of a cable from reflectometry measurements made at both ends of the cable. It enables detection, localization and estimation of dissipative soft-faults. In this reported work, we address the problem of impedance mismatch between the measurement instrument and the cable, based on a pre-processing of the measured data before running the estimation computations. It aims at reducing the impedance mismatch between instrumentation and the cable under test without physical intervention on the test fixtures. In addition, a measurement procedure has been developed

in order to get the two-ends reflectometry measurements without actually connecting both ends of the cable under test to a single instrument [25].

## 7.7. Sensor and hardware based research

## 7.7.1. Cracks detection in pavement by a distributed fiber optic sensing technology

Participant: Xavier Chapeleau.

This paper presents the feasibility of damage detection in asphalt pavements by embedded fiber optics as a new non-destructive inspection technique. The distributed fiber optic sensing technology based on the Rayleigh scattering was used in this study. The main advantage of this technique is that it allows to measure strains over a long length of fiber optic with a high spatial resolution, less than 1 cm. By comparing strain profiles measured at different times, an attempt was made to link strain changes with the appearance of damage (cracking) in the pavement. This non-destructive method was evaluated on accelerated pavement testing facility, in a bituminous pavement. In our experimentation, the optical fibers were placed near the bottom of the asphalt layer. The application of 728 000 heavy vehicle loads (65 kN dual wheel loads) was simulated in the experiment. Optical fiber measurements were made at regular intervals and surface cracking of the pavement was surveyed. After some traffic, a significant increase of strains was detected by the optical fibers at different points in the pavement structure, before any damage was visible. Later, cracking developed in the zones where the strain profiles were modified, thus indicating a clear relationship between the increased strains and crack initiation. These first tests demonstrate that distributed fiber optic sensors based on Rayleigh scattering can be used to detect crack initiation and propagation in pavements, by monitoring strain profiles in the bituminous layers [17].

### 7.7.2. Wireless sensors and GPS synchronization

Participants: Vincent Le Cam, David Pallier.

Most of recent development in WSN domain focused on energy (saving or harvesting), on wireless protocols, on embedded algorithms. But it is a fact that, most of monitoring applications need samples to be timestamped. According to the application, the wished time resolution could be up to one second for automation monitoring, one millisecond for vibration, one microsecond for acoustic monitoring, one nanosecond for electricity or light propagation... The consequence for a Wireless network of electronic nodes is that, by nature, no common signal could physically provide a synchronization top. But, as each electronic device, a wireless sensor time-base uses a timer incremented by a quartz whose initial value is theoretical up to some p.p.m. and whose period drift on time because of age, temperature,... Two kind of solutions could be regarded : a synchronization signal provided by the wireless protocol itself; an absolute synchronization from a referential source such as: GPS, Frankfurt clock, Galileo,... In the first way, it will be demonstrated the poor accuracy and the need of energy such a mechanism offers. In the second way, the article will details how a deterministic (Universal Time), accurate and resilient algorithm has been implemented. The article also provides specific results of application on acoustic monitoring system and electricity propagation where the accuracy of a WSN has reached up to 10 nanosecond UT. Consequence on energy consumption of this algorithm are given with a description of future works to improve the energy balance while keeping the device sober and synchronized [33].

## **MCTAO Project-Team**

## 6. New Results

## 6.1. Stability properties of geodesic flows on Riemannian manifolds

Participants: Ludovic Rifford, Rafael Ruggiero [PUC, Rio de Janeiro, Brazil].

In a paper by Rifford and Ruggiero [25], the  $C^2$ -structural stability conjecture from Mañé's viewpoint for geodesics flows of compact manifolds without conjugate points is investigated. The structural stability conjecture is an open problem in the category of geodesic flows because the  $C^1$  closing lemma is not known in this context. Without the  $C^1$  closing lemma, we combine the geometry of manifolds without conjugate points and a recent version of Franks' Lemma from Mañé's viewpoint to prove the conjecture for compact surfaces, for compact three dimensional manifolds with quasi-convex universal coverings where geodesic rays diverge, and for *n*-dimensional, generalized rank one manifolds.

## 6.2. Optimal transport and sub-Riemannian geometry

## 6.2.1. Uniquely minimizing costs for the Kantorovitch problem

**Participants:** Ludovic Rifford, Robert Mccann [Univ of Toronto, Canada], Abbas Moameni [Carleton Univ, Ottawa, Canada].

In continuation of the work by McCann and Rifford [65], a paper by Moameni and Rifford [24] study some conditions on the cost which are sufficient for the uniqueness of optimal plans (provided that the measures are absolutely continuous with respect to the Lebesgue measure). As a by-product of their results, the authors show that the costs which are uniquely minimizing for the Kantorovitch problem are dense in the  $C^0$ -topology. Many others applications and examples are investigated.

## 6.2.2. The Sard conjecture in sub-Riemannian geometry, optimal transport and measure contraction properties

Participants: Zeinab Badreddine, Ludovic Rifford.

Zeinab Badreddine [13] obtained the first result of well-posedness for the Monge problem in the sub-Riemannian setting in the presence singular minimizing curves. This study is related to the so-called measure contraction property. In collaboration with Rifford [14], Badreddine obtained new classes of sub-Riemannian structures satisfying measure contraction properties.

## 6.3. Optimal control of fully actuated micro-swimmers

### 6.3.1. A general geometric approach of optimal strokes for driftless micro-swimmers

Participants: Thomas Chambrion [Univ. Lorraine], Laetitia Giraldi, Alexandre Munnier [Univ. Lorraine].

In [3], we study the control problem associated to the locomotion of a deformable swimmer. we present a unified geometric approach for optimization of the body deformation of the swimmers in a 3D Stokes flow (case of micro-swimmers) and 2D or 3D potential flow. The latter cases correspond to the analysis of the sphere in a sub-Riemannian space. A general framework is introduced, allowing the complete analysis of five usual nonlinear optimization problems to be carried out. The results are illustrated with examples and with a in-depth study of a swimmer in a 2D potential flow. Numerical tests are also provided.

## 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 [43], this model describes 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 contribution is 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, see [16]. 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) and K. Sérier's PhD (started September, 2017), see [10], [42] and other publications under review.

## 6.4. Modelling and controllability of Magneto-elastic Micro-swimmers

## 6.4.1. Purcell magneto-elastic swimmer controlled by an external magnetic field

**Participants:** François Alouges [École Polytechnique], Antonio Desimone [SISSA Trieste, Italy], Laetitia Giraldi, Marta Zoppello [Univ. di Padova, Italy].

We have studied the mechanism of propulsion of a Purcell swimmer whose segments are magnetized and react to an external magnetic field applied into the fluid. By an asymptotic analysis, we prove that it is possible to steer the swimmer along a chosen direction when the control functions are prescribed as an oscillating field. Moreover, there are obstructions that have to be overcome in order to get classical controllability result for this system. This is exposed in [7] (IFAC World Congress, Toulouse, July 2017).

### 6.4.2. Local Controllability of the Two-link Magneto-elastic Micro-swimmer

Participants: Laetitia Giraldi, Pierre Lissy [Univ. Paris Dauphine], Clément Moreau, Jean-Baptiste Pomet.

For the smallest magneto-elastic micro-swimmer (2 links), we have been able to prove a strong local controllability result around its straight position of the swimmer. This is exposed in[6]. However, the latter result is weaker than the classical local controllability concept called STLC which means that a system could reach any position around its equilibrium with a small control (as small as the desired displacement of the system). Moreover, we prove in [5] that the 2-link magneto-elastic swimmer is indeed *not* STLC.

## 6.5. Numerical aspect of the N-link micro-swimmer model

Participants: Hermes Gadhêla [Univ. of York, UK], Laetitia Giraldi, Clément Moreau, Jean-Baptiste Pomet.

This topic was initiated with a 1 year research invitation of Clément Moreau at University of York and further collaboration. The goal is to compare the ODE given by the "*N*-link swimmer" model with the PDE for an elastic rod.

In [22], we study inertialess fluid-structure interaction of active and passive inextensible filaments. In this work, we compare two different approaches that lead to model the behavior of a microscopic elastic filament immersed into a fluid. The first which derives from a continuous formalism corresponds to solve a PDE, the second method exploits the momentum balance in the asymptotic limit of small rod-like elements which are integrated semi-analytically. The equivalence between the continuous and asymptotic model allows a direct comparison between the two formalisms. The asymptotic model is simple and intuitive to implement, and generalisations for complex interaction of multiple rods. We demonstrate these via four benchmarks: transient dynamics, force-displacement buckling instability, magnetic artificial swimmer and cross-linked filament-bundle dynamics.

## 6.6. Optimal Control and Averaging in Aerospace Engineering

## 6.6.1. Chance-constrained optimal control problems in aerospace

**Participants:** Jean-Baptiste Caillau, Max Cerf [Airbus Safran Launchers], Achille Sassi [ENSTA Paristech], Emmanuel Trélat [Univ. Paris VI], Hasnaa Zidani [ENSTA Paristech].

The aim is to minimize the fuel mass of the last stage of a three-stage launcher. Since the design parameters of the spacecraft are not exactly known prior to the launch, uncertainties have to be taken into account. Although these parameters are supposed to be uniformly distributed on fixed ranges, it is not desirable to use "worstcase" robust optimization as the problem may not even be feasible for some values of the parameters due to very strong sensitivities. The idea is to frame instead a stochastic optimization problem where these parameters are independent stochastic variables. The original constraint becomes a stochastic variable, and one only asks that the desired target is reached with some given probability. A key issue in solving this chance constrained problem is to approximate the probability density function of the constraint. Contrary to Monte-Carlo methods that require a large number of runs, kernel density estimation [68] has the strong advantage to permit to build an estimator with just a few constraint evaluations. This approach allows to treat efficiently uncertainties on several design parameters of the launcher, including the specific impulse and index of the third stage and using a simple affine discretization of the control (pitch angle). In [19], 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, and we show how this technique can be applied and implemented for a class of problems including the Goddard problem (with bang-bang or bang-singular-bang controls) and the trajectory optimization of an Ariane 5-like launcher. This work has been done in collaboration with Airbus Safran Launchers at Les Mureaux.

An involved question in chance constrained optimization is the existence and computation of the derivative of the stochastic constraint with respect to deterministic parameter. This shall be investigated in the light of new results in the Gaussian case [78]. Using a single deterministic control to reach a given target (or a given level of performance) with some fixed probability when the parameters of the system are randomly distributed is very similar to issues of ensemble controllability addressed in the recent work [26]. One expects some insight from the comparison of the two viewpoints.

### 6.6.2. Metric approximation of minimum time control systems

Participants: Jean-Baptiste Caillau, Lamberto Dell'Elce, Jean-Baptiste Pomet, Jérémy Rouot.

Slow-fast affine control systems with one fast angle are considered in this work [20]. An approximation based on standard averaging of the extremal is defined. When the drift of the original system is small enough, this approximation is metric, and minimum time trajectories of the original system converge towards geodesics of a Finsler metric. The asymmetry of the metric accounts for the presence of the drift on the slow part of the original dynamics. The example of the  $J_2$  effect in the two-body case in space mechanics is examined. A critical ratio between the  $J_2$  drift and the thrust level of the engine is defined in terms of the averaged metric. The qualitative behaviour of the minimum time for the real system is analyzed thanks to this ratio. Work in progress aims at dealing with multiphase averaging for systems driven by several fast angles.

#### 6.6.3. Approximation by filtering in optimal control and applications

**Participants:** Jean-Baptiste Caillau, Thierry Dargent [Thales Alenia Space], Florentina Nicolau [Univ. Cergy-Pontoise].

Minimum time control of slow-fast systems is considered in this analysis [8]. In the case of only one fast angle, averaging techniques are available for such systems. The approach introduced in [57] and [34] 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 motivation is that averaging over an entire period may not provide a good enough approximation to initialize a convergent numerical resolution of the original system; considering a continuous

set of intermediate approximations (filtering over windows of size varying from the period to zero) may ensure convergence. The method is illustrated on problems coming from space mechanics and has been implemented as an addition to the industrial code T3D of Thales Alenia Space.

## 6.6.4. Higher order averaging

**Participants:** Jean-Baptiste Pomet, Thierry Dargent [Thales Alenia Space], Florentina Nicolau [Univ. Cergy-Pontoise].

A further step in defining a suitable approximation of slow-fast oscillating controlled systems is to go beyond the  $O(\varepsilon)$  uniform error provided by simple averaging. An original approach has been proposed in [58] and demonstrated numerically; it consists in correcting the boundary values of the slow averaged variables to ensure an  $O(\varepsilon^2)$  average error, without the difficulties of classical second order averaging [73] (that leads to an  $O(\varepsilon^2)$  uniform error, that we do not need), and allows an  $O(\varepsilon)$  approximation of the angle. It is proved in [9] that it is indeed possible, at least for initial value problems, to compute order one corrections of the initial slow variables to guarantee such an error. From the numerical side, this process is a key to be able to initialize shooting methods on the non-averaged system by averaged solutions when using a model with full perturbations in orbit transfer.

## 6.7. Stability of nonlinear high frequency amplifiers

**Participants:** Sébastien Fueyo, Jean-Baptiste Pomet, Laurent Baratchart [APICS project-team APICS (FAC-TAS as of 2018)].

Sébastien Fueyo's PhD is co-advised between McTAO and APICS on this topic. The problem is presented in section 4.4.

Starting from infinite dimensional time-domain models for these devices, we obtained full justification (with some possible obstructions) to the prediction of stability through transfer function identification on academic examples of simple circuits, and are working on generalisations. A preliminary presentation will be given at a local conference, Université Côte d'Azur Complex Days, in January, 2018.

## **NECS Project-Team**

## 7. New Results

## 7.1. Networks: modeling, analysis and estimation

### 7.1.1. 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. We study linear network systems, and we aim at characterizing input and state observability (ISO), namely the conditions under which both the whole network state and the unknown input can be reconstructed from some measured local states. We complement the classical algebraic characterizations with novel structural results, which depend only on the graph of interactions (equivalently, on the zero pattern of the system matrices). More precisely, there are two kinds of results: structural results, true for almost all interaction weights, and strongly structural results, true for all non-zero interaction weights.

In [32], we consider linear time-invariant (LTI) systems, for which we provide a full characterization of structural ISO. The characterization of strongly structural ISO is on-going work.

In [33], instead, we consider linear time-varying (LTV) systems, under some assumptions on the input and output matrices, namely that each attack input and each output measurement concerns a single local state, and that there is no direct feedthrough of the input to the output. Under these assumptions, we characterize strongly structural ISO; in [23] we also give the characterization of structural ISO under the same assumptions.

We are currently working on analogous characterizations for the more general case, removing these assumptions.

Observability is also related to privacy issues. In the ProCyPhyS project, started in 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. Precisely, by assuming scenarios where nodes compute an average of their initial condition in a finite number of steps with have state privacy-preserving conditions and devise a simple policy that guarantee privacy in case of observable networks.

#### 7.1.2. Sensor networks: multisensor data fusion for navigation

Participants: H. Fourati [Contact person], T. Michel.

Attitude estimation consists in the determination of rigid body orientation in 3D space (principally in terms of Euler angles, rotation matrix, or quaternion). In [27], we solved the attitude determination problem based on a single sensor observation. The rotation equation is transformed into a quadratic quaternion form and is then derived to a linear matrix equation with pseudoinverse matrices. The analytic solutions to the equation are computed via elementary row operations. The solutions show that the attitude determination from a single sensor observation has infinite solutions and the general one is governed by two limiting quaternions. Accordingly, the variance analysis is given in view of probabilistic characters. The authors explore the experimental results via the accelerometer attitude determination system. The properties of the two limiting quaternions are investigated in the experiment. The results show that the gravity-determination abilities of the two limiting quaternions are quite different. Using the rotation vector and eigenvalue decomposition of the

attitude matrix, the authors prove that one limiting quaternion is better than another one geometrically. The singularity analysis is also performed revealing the non-existence of singularities for limiting quaternions. The above findings are novel, which are quite different from the conclusions made in a previously published study. In [26], we presents a novel linear approach to solve this problem. We name the proposed method the Fast Linear Attitude Estimator (FLAE) because it is faster than known representative algorithms. The original Wahba's problem is extracted to several 1-dimensional equations based on quaternions. They are then investigated with pseudo-inverse matrices establishing a linear solution to n-dimensional equations, which are equivalent to the conventional Wahba's problem. To obtain the attitude quaternion in a robust manner, an eigenvalue-based solution is proposed. Symbolic solutions to the corresponding characteristic polynomial is derived showing higher computation speed. Simulations are designed and conducted using test cases evaluated by several classical methods e.g. M. D. Shuster's QUaternion ESTimator (QUEST), F. L. Markley's SVD method, D. Mortari's Second Estimator of the Optimal Quaternion (ESOQ2) and some recent representative methods e.g. Y. Yang's analytical method and Riemannian manifold method. The results show that FLAE generates attitude estimates as accurate as that of several existing methods but consumes much less computation time (about 50% of the known fastest algorithm). Also, to verify the feasibility in embedded application, an experiment on the accelerometer-magnetometer combination is carried out where the algorithms are compared via C++ programming language. An extreme case is finally studied, revealing a minor improvement that adds robustness to FLAE. We have been interested in other work [28] to some critical issues on Kalman filter observed in navigation solutions of Global Navigation Satellite System (GNSS). The Kalman filtering (KF) is optimal under the assumption that both process and observation noises are independent white Gaussian noise. However, this assumption is not always satisfed in real-world navigation campaigns. In this paper, two types of KF methods are investigated, i.e. augmented KF (AKF) and the second moment information based KF (SMIKF) with colored system noises, including process and observation noises. As a popular noise-whitening method, the principle of AKF is briefly reviewed for dealing with the colored system noises. The SMIKF method is developed for the colored and correlated system noises, which directly compensates for the covariance through stochastic model in the sense of minimum mean square error. To accurately implement the SMIKF, a refned SMIKF is further derived regarding the continuous-time dynamic model rather than the discrete one. The computational burdens of the proposed SMIKF along with representative methods are analyzed and compared. The simulation results demonstrate the performances of proposed methods.

#### 7.1.3. Network reduction towards a scale-free structure preserving physical properties

Participants: N. Martin, P. Frasca, C. Canudas de Wit [Contact person].

In the context of the ERC project, we are addressing a problem of graph reduction, where a given arbitrary weighted graph is reduced to a (smaller) scale-free graph while preserving a consistency with the initial graph and some physical properties. This problem can be formulated as a minimization problem. We give specifications to this general problem to treat a particular case: to this end we define a metric to measure the scale-freeness of a graph and another metric to measure the similarity between two graphs with different dimensions, based on a notion of spectral centrality. Moreover, through the reduction we also preserve a property of mass conservation (essentially, Kirchoff's first law). We study the optimization problem and, based on the gained insights, we derive an algorithm allowing to find an approximate solution. Finally, we have simulated the algorithm both on synthetic networks and on real-world examples of traffic networks that represent the city of Grenoble.

## 7.1.4. The Observability Radius of Networks

Participants: G. Bianchin, P. Frasca [Contact person], A. Gasparri, F. Pasqualetti.

Our group is undergoing an effort to understand the system-theoretic properties of networks, namely in terms of controllability and observability. In this context, we have studied the observability radius of network systems, which measures the robustness of a network to perturbations of the edges. We consider linear networks, where the dynamics are described by a weighted adjacency matrix and dedicated sensors are positioned at a subset of nodes. We allow for perturbations of certain edge weights with the objective of

preventing observability of some modes of the network dynamics. To comply with the network setting, our work considers perturbations with a desired sparsity structure, thus extending the classic literature on the observability radius of linear systems. The paper [14] proposes two sets of results. First, we propose an optimization framework to determine a perturbation with smallest Frobenius norm that renders a desired mode unobservable from the existing sensor nodes. Second, we study the expected observability radius of networks with given structure and random edge weights. We provide fundamental robustness bounds dependent on the connectivity properties of the network and we analytically characterize optimal perturbations of line and star networks, showing that line networks are inherently more robust than star networks.

#### 7.1.5. Distributed Estimation from Relative and Absolute Measurements

Participants: P. Frasca [Contact person], W.s. Rossi, F. Fagnani.

Important applications in machine learning, in robotic coordination and in sensor networks require distributed algorithms to solve the so-called relative localization problem: a node-indexed vector has to be reconstructed from measurements of differences between neighbor nodes. In [22] we define the problem of least-squares distributed estimation from relative and absolute measurements, by encoding the set of measurements in a weighted undirected graph. The role of its topology is studied by an electrical interpretation, which easily allows distinguishing between topologies that lead to "small" or "large" estimation errors. The least-squares problem is solved by a distributed gradient algorithm, which we have studied in detail. Remarkably, we have observed that the computed solution is approximately optimal after a number of steps that does not depend on the size of the problem or on the graph-theoretic properties of its encoding. This fact indicates that only a limited cooperation between the sensors is necessary to solve this problem.

## 7.2. Multi-agent systems and network games

## 7.2.1. 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 concerned the complexity of the best response algorithm under round-robin revision sequence, a classical centralized iterative algorithm to find a Nash Equilibrium. In a more recent work, submitted for publication, and described in the report [40], we focus on distributed versions of the same algorithm. We compute the average complexity over all potential games of best response dynamics under a random i.i.d. revision sequence, since it can be implemented in a distributed way using Poisson clocks. We obtain a distributed algorithm whose execution time is within a constant factor of the optimal centralized one. We then show how to take advantage of the structure of the interactions between players in a network game: noninteracting players can play simultaneously. This improves best response algorithm, both in the centralized and in the distributed case.

## 7.2.2. Using a linear gain to accelerate average consensus over unreliable networks

Participants: F. Acciani, P. Frasca [Contact person], G. Heijenk, A. Stoorvogel.

Packet loss is a serious issue in wireless consensus networks, as even few failures might prevent a network to converge to the desired consensus value. In some recent work, we have devised a possible way to compensate for the errors caused by packet collisions, by modifying the updating weights. Such a modification compensates for the loss of information in an unreliable network, but results in a reduced convergence speed. In [30], we propose a faster method - based on a suitable gain in the consensus dynamics - to solve the unreliable average consensus problem. We find a sufficient condition for the gain to preserve stability of the network. Simulations are used to discuss the choice of the gain, and to compare our method with the literature.

## 7.2.3. Mean-field analysis of the convergence time of message-passing computation of harmonic influence in social networks

Participants: W. S. Rossi, P. Frasca [Contact person].

In the study of networks, identifying the most important nodes is of capital importance. The concept of Harmonic Influence has been recently proposed as a metric for the importance of nodes in a social network. This metric evaluates the ability for one node to sway the 'opinions' of the other nodes in the network, under the assumption of a linear diffusion of opinions in the network. A distributed message passing algorithm for its computation has been proposed by Vassio et al., 2014, and proved to converge on general graphs by Rossi and Frasca, 2016. In [36], we presented an want to evaluate the convergence time of this algorithm by using a mean-field approach. The mean-field dynamics is first introduced in a "homogeneous" setting, where it is exact, then heuristically extended to a non-homogeneous setting. The rigorous analysis of the mean-field dynamics is complemented by numerical examples and simulations that demonstrate the validity of the approach.

#### 7.2.4. Modeling birds on wires

**Participants:** A. Aydogdu, P. Frasca [Contact person], C. d'Apice, R. Manzo, J. M. Thornton, B. Gachomo, T. Wilson, B. Cheung, U. Tariq, W.m. Saidel, B. Piccoli.

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

## 7.2.5. Network Games: Condensation of the Graph as a Hierarchical interpretation of the Game

Participants: G. Casadei, C. Canudas de Wit [Contact person].

Control and optimization over large population networks have become a popular topic within the control community. The main reason is that modern applications re- quire multiple systems to communicate and interact with each other to fulfill the desired task. For instance power networks, sensor networks and social networks are solid examples in which is fundamental to control different parts of the network to achieve a global desired behavior. In the recent years, the control community has largely focused on cooperative approaches to networks. In this framework the agents in the network are willing to collaborate and find an agreement between each other in such a way that they coordinate their motion.

However, not in all the frameworks and not in all the situations, it is possible to consider a cooperative approach. In several scenarios, the nodes are selfish and in competition with the others to pursue their goal. This leads to a non-cooperative interaction between the agents and thus to games played over networks. When the number of nodes in the network is large, it becomes analytically impossible to use conventional game theoretic tools to find a solution to the problem. This motivated researchers to define a new type of games, named aggregative, where the response of an agent depends, rather than on each other players decision, on the aggregation of all the other agents action.

We considered a refined typology of networks games in which the aggregate information is depending on a directed communication graph and showed that under a certain number of conditions the players reach a Nash Equilibrium. Then we study the influence of this graph topology on the structure of the game and show that the condensation of the graph leads to a hierarchical interpretation of the game and thus to a quasi-sequential architecture of optimization. Then, we introduce the concept of physical graph and control graph in flow networks, and show that the condensation of the control graph helps in determining the equilibrium the agents will reach.

## 7.3. Transportation networks and vehicular systems

## 7.3.1. Travel time prediction

Participants: A. Kibangou [Contact person], H. Fourati, C. Canudas de Wit, A. Ladino, M Rodriguez.

One of the regular performance metrics for qualifying the level of congestion in traffic networks is the travel time. In [24], we addressed the problem of dynamic travel time (DTT) forecasting within highway traffic networks using speed measurements. 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 a predictor computationally simple to be implemented. To take into account the lack of information in the cluster assignment for the new predicted values, a weighted average fusion based on a similarity measurement 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. We consider in a recent paper submitted to European Control Conference 2018 the problem of joint reconstruction of flow and density in a urban traffic network using heterogeneous sources of information. The traffic network is modeled within the framework of macroscopic traffic models, where we adopt Lighthill-Whitham-Richards model (LWR) conservation equation and a piecewise linear fundamental diagram. The estimation problem considers three key principles. First, the principle governing traffic models where flow is maximized in a junction. Second, the error minimization between the measured and reconstructed flows and velocities, and finally the equilibrium state of the network which establishes flow propagation within the network. All principles are integrated and the problem is casted as a constrained quadratic optimization with inequality and equality constraints in order to shrink the feasible region of estimated variables. Some simulation scenarios based on synthetic data for a Manhattan grid network are provided in order to validate the performance of the proposed algorithm.

## 7.3.2. Urban traffic control

Participants: C. Canudas de Wit [Contact person], F. Garin, P. Grandinetti.

The PhD thesis of Pietro Grandinetti 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, together with balancing densities across the network. 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. A modified version of the algorithm uses simplified optimization (purely local, instead of distributed) but takes into account the real constraints in Grenoble downtown traffic lights network, such as priority to public transportation, and imposed minimal and maximal green duration, leading to a fully realistic implementation, tested using Aimsun microscopic simulator.

## 7.3.3. Traffic Regulation Via Controlled Speed Limit

Participants: M. L. Delle Monache [Contact person], B. Piccoli, F. Rossi.

The work [21] address the speed limit problem on a single road. The control variable is the maximal allowed velocity, which may vary in time but we assume to be of bounded total variation, and we aim at tracking a given target outgoing flow. More precisely, the main goal is to minimize the quadratic difference between the achieved outflow and the given target outflow. Mathematically the problem is very hard, because of the delays in the effect of the control variable (speed limit). In fact, the link entering time, which represents the entering time of the car exiting the road at time t, depends on the given inflow and the control policy on the whole time interval. Moreover, the input-output map is defined in terms of the Link Entering Time, thus the achieved outflow at time t depends on the control variable on the whole time interval. After formulating the optimal control problem, we consider needle-like variations for the control policy as used in the classical Pontryagin maximum principle. We are able to derive an analytical expression of the one-sided variation of the cost, corresponding to needle-like variations of the control policy, using

fine properties of functions with bounded variation. In particular the one-sided variations depend on the sign of the control variation and involve integrals w.r.t. the distributional derivative of the solution as a measure. This allows us to prove Lipschitz continuity of the cost functional in the space of a bounded variation function and prove existence of a solution. Afterwards, we define three different techniques to numerically solve this problem and we compare the three approaches on two test cases.

#### 7.3.4. Scalar conservation laws with moving flux constraints

Participants: M. L. Delle Monache [Contact person], P. Goatin [Acumes, Inria], C. Chalons.

This problem is motivated by the modeling of a moving bottleneck in traffic flow, which can be caused by a large, slow moving vehicle. A slow moving large vehicle, like a bus or a truck, reduces the road capacity and thus generates a moving bottleneck for the surrounding traffic flow. This situation can be modeled by a PDE–ODE strongly coupled system consisting of a scalar conservation law with moving flux constraint accounting for traffic evolution and an ODE describing the slower vehicle motion. In [18], we introduce a novel approach to solve numerically this problem. The main point here is related to the presence of non-classical shocks in the solutions of the model under consideration. It is well-known that, in this context, standard conservative finite volume methods cannot be applied and fail in producing good numerical results. Glimm's scheme can be used but it is not strictly conservative. In order to propose a numerical scheme which is conservative on fixed meshes and able to compute non-classical solutions, we propose to adapt a reconstruction strategy approach, which allows to precisely capture moving non-classical discontinuities on fixed meshes still guaranteeing conservation, unlike Glimm's scheme. An important feature of the proposed method is to be exact for isolated classical and non-classical shocks, which means in particular only one point of numerical diffusion (on each cell the approximate value corresponds to the value of the average of the exact solution). In the general case, shocks are still computed without numerical diffusion and convergence is proved numerically.

In [19] we study well-posedness of a scalar conservation laws with moving flux constraints. In this work we assume that the constraint trajectory is given and it does not depend on the solution of the PDE. In this setting we then show Lipschitz continuous dependence of bounded variation solutions with respect to the initial data and the constraint trajectory.

## 7.3.5. Priority-based Riemann solver for traffic flow on networks

Participants: M. L. Delle Monache [Contact person], P. Goatin [Acumes, Inria], B. Piccoli.

In [20] we introduce a novel solver for traffic intersection which considers priorities among the incoming roads as the first criterion and maximization of flux as the second. The main idea is that the road with the highest priority will use the maximal flow taking into account also outgoing roads constraints. If some room is left for additional flow then the road with the second highest priority will use the left space and so on. A precise definition of the new Riemann solver, called Priority Riemann Solver, is based on a traffic distribution matrix, a priority vector and requires a recursion method. The general existence theorem for Riemann solvers on junctions can not be applied in the present case. Therefore, we achieve existence via a new set of general properties.

## 7.3.6. Discrete-time system optimal dynamic traffic assignment (SO-DTA) with partial control for horizontal queuing networks

**Participants:** S. Samaranayake, J. Reilly, W. Krichene, M. L. Delle Monache [Contact person], P. Goatin [Acumes, Inria], A. Bayen.

Dynamic traffic assignment (DTA) is the process of allocating time-varying origin-destination (OD) based traffic demand to a set of paths on a road network. There are two types of traffic assignment that are generally considered, the user equilibrium or Wardrop equilibrium allocation (UE-DTA), in which users minimize individual travel-time in a selfish manner, and the system optimal allocation (SODTA) where a central authority picks the route for each user and seeks to minimize the aggregate total travel-time over all users. It can be shown that the price of anarchy (PoA), the worst-case ratio of the system delay caused by the selfish behavior over the system optimal solution, may be arbitrarily large even in simple networks. System optimal (SO) traffic assignment on the other hand leads to optimal utilization of the network resources, but is hard to achieve in practice since the overriding objective for individual drivers in a road network is to minimize their own travel-time. It is well known that setting a toll on each road segment corresponding to the marginal delay of the demand moves the user equilibrium towards a SO allocation. In [25], we formulate the system optimal dynamic traffic assignment problem with partial control (SO-DTAPC), using a Godunov discretization of the Lighthill-Williams-Richards (LWR) partial differential equation (PDE) with a triangular flux function. We propose solving the SO-DTA-PC problem with the non-convex traffic dynamics and limited OD data with complete split ratios as a non-linear optimal control problem. This formulation generalizes to multiple sources and multiple destinations. We show that the structure of our dynamical system allows for very efficient computation of the gradient via the discrete adjoint method.

## 7.3.7. Measuring trajectories and fuel consumption in oscillatory traffic: experimental results

Participants: F. Wu, R. Stern, M. Churchill, M. L. Delle Monache [Contact person], K. Han, B. Piccoli.

In [37] we present data collected through a set of experiments with nine to 10 vehicles driving on a ring road constructed on a closed track. Vehicle trajectory data is extracted via a series of vision processing algorithms (for background subtraction, vehicle identification, and trajectory extraction) from a 360-degree panoramic camera placed at the center of the ring. The resulting trajectory data is smoothed via a two-step algorithm which applies a combination of RLOESS smoothing and regularized differentiation to produce consistent position, velocity, and acceleration data that does not exhibit unrealistic accelerations common in raw trajectory data extracted from video. A subset of the vehicles also record real-time fuel consumption data of the vehicles using OBD-II scanners. The tests include both smooth and oscillatory traffic conditions, which are useful for constructing and calibrating microscopic models, as well as fuel consumption estimates from these models. The results show a an increase in fuel consumption in the experiments in which traffic oscillations are observed as compared to experiments where vehicles maintain a smooth ow. However, this is partially due to the higher average speed at which vehicles travel in the experiments in which oscillatory traffic is observed. The article contains a complete, publicly available dataset including the video data, the extracted trajectories, the smoothed trajectories, and the OBD-II logs from each equipped vehicle. In addition to the dataset, this article also contains a complete source code for each step of the data processing. It is the first of several experiments planned to collect detailed trajectory data and fuel consumption data with smooth and unsteady traffic flow in a controlled experimental environment.

## 7.3.8. Large Scale Traffic Networks and Aggregation

Participants: G. Casadei, V. Bertrand, B. Gouin, C. Canudas de Wit [Contact person].

Large scale traffic networks are a popular topic nowadays due to the impact traffic has in our everyday life, both economically and health-wise. City management are interested in understanding the evolution of traffic and its patterns over the city in order to take decision on potential changes and to design new and more functional infrastructure. However, monitoring the current state of a large scale traffic network is a demanding task. The heterogeneity of available measures poses several question on how to merge different sources of information coming from private and public sources. Furthermore, sparsity is an intrinsic issues related to

large scale systems: independently from the source we choose to rely on, we cannot expect the measurements to be sufficiently dense to cover the full network in detail.

For large scale urban network, managing real-time traffic information from thousands of links simultaneously is an overwhelming task and extracting interesting and meaningful insights from these tangle of data can be even a more challenging aim. In recent years more and more data are becoming available from new sources, such as smart phones, GPS navigators, and their technological penetration nowadays allows to have an impressive amount of real-time traffic information, not requiring the placement of physical sensors over the network and thus reducing incredibly costs due to installation and maintenance: in other words, each user becomes a moving sensor inside the network.

One way to deal with this huge amount of data over a urban traffic network is to look at the graph describing the network with a clusterization approach: this would reduce the number of nodes, thus the computational cost, proportionally to the clusterization rate and potentially would help with sparsity by merging areas in which no data are available with areas with sufficient penetration of information. In this work we presented an aggregation-based technique to analyze GPS velocity data from a private source (TomTom) and to calculate multi-origin multi-destination travel time. The technique we propose allows to perform the aggregation and the necessary computation in such a way that its application in a real time framework is feasible. The information and results we obtain are of great interest to understand the macroscopic evolution of the traffic from a large-scale point of view and to evaluate the average time that users spend in transiting between different areas along the day. In practice, we show that reducing the *complexity* of the network by 95% thanks to aggregation, we introduce an error in the calculation of the traveling times that in the average is below 25%.

### 7.3.9. Two dimensional models for traffic

Participants: S. Mollier, M. L. Delle Monache, C. Canudas de Wit [Contact person].

The work deals with the problem of modeling traffic flow in urban area, e. g. a town. More precisely, the goal is to design a two-dimensional macroscopic traffic flow model suitable to model large network as the one of a city. Macroscopic traffic models are inspired from fluid dynamic. They represent vehicles on the road by a density and describe their evolution with partial differential equations. Usually, these models are one dimensional models and, for instance, give a good representation of the evolution of traffic states in highway. The extension of these 1D models to a network is possible thanks to models of junction but can be tedious according to the number of parameters to fit. In the last few years, the idea of models based on a two dimensional conservation laws arose in order to represent traffic flow in large and dense networks. This study aims to develop such models with new designs especially including the network topology, and validation with simulation.

## **NON-A Project-Team**

## 7. New Results

## 7.1. Research axis 1: General annihilators (tools: ALG)

- Integro-differential equations and integro-differential algebras were studied in [91], presenting new opportunities in nonlinear control theory.
- Algebraic estimation in partial derivatives systems were studied in [93].
- An effective version of the algebraic parameter estimation problem has recently been initiated in [73] based on algebraic analysis (module theory, homological algebra) and computer algebra (differential elimination techniques, Gröbner basis methods for noncommutative polynomial rings of ordinary differential operators with polynomial coefficients). The results of [73] have been implemented in the Maple package NonA built upon the package OreModules.

# 7.2. Research axis 2: Numerical differentiation and finite-time estimation (tools: HOM)

- Algorithms of finite-time and fixed-time observer design have been developed for linear plants based on Implicit Lyapunov function method and homogeneity [30].
- In [23], 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 nonzero degrees, whereas the implicit Euler scheme ensures convergence of the approximating solutions to zero. Properties of absolute and relative errors of the respective discretizations are investigated.
- In [34], the problem of time-varying parameter identification is studied. To this aim, two identification algorithms are developed in order to identify time-varying parameters in a finite-time or prescribed time (fixed-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-based approach. The results are obtained under injectivity of the regressor term, which is related to the classical identifiability condition. The case of bounded disturbances (noise of measurements) is analyzed for both algorithms. Simulation results illustrate the feasibility of the proposed algorithms.
- [36] contributes to the stability analysis for nonlinear impulsive dynamical systems based on a vector Lyapunov function and its divergence operator. The new method relies on a 2D time domain representation. Different types of stability notions for a class of nonlinear impulsive systems are studied using a vector Lyapunov function approach. The results are applied to analyze the stability of a class of Lipschitz nonlinear impulsive systems based on Linear Matrix Inequalities. Some numerical examples illustrate the feasibility of the proposed approach.
- [21] 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.

- [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.
- Delay estimation algorithms based on sliding mode methodology have been presented in [44].
- A nonlinear distributed observer was proposed in [81] for the problem of distributed estimation in a linear large-scale system.
- In [15], we analyze the observability for linear singular systems with delays, and the corresponding observer design technique has been proposed in [42]. For nonlinear singular system without delay, we propose in [43] a nonlinear Luenberger-like observer. For systems with delays, in [44], we investigate the identifiability of time-delay, and use a sliding mode technique and a classical Newton method to estimate the delay.

# 7.3. Research axis 3: Control without sophisticated models (tools: ALG-HOM-SET)

- Topological equivalence between quadratically stable and homogeneous asymptotically stable systems have been proven in [72].
- Boundary finite-time control for heat system have been developed in [69], but hyper-exponential control for state delay linear systems have been developed in [70].

## 7.4. Research axis 4: Applications (tools: ALG-HOM-SET)

- Robust set-point tracking control and optimal control algorithms for turbulent flows have been developed in [26] and tested in Wind Tunnel L1 of ONERA, Lille. (https://www.youtube.com/watch?v=b5NnAV2qeno) The set-point tacking control have been patented, FR 1755440, "Dispositif de contrôle actif du recollement d'un écoulement sur un profil".
- In [75], [77], the development of a robust  $(H_{\infty})$  control for parametric systems has been initiated. A general framework based on symbolic computation techniques was proposed. In these two papers, the general approach has been applied to the case of linear systems of order up to four and illustrated with the two mass-spring system with damping. In particular, closed forms for the robust controllers and for the robustness radius were obtained. Finally, the robust stabilization of the line of sight of a stabilized mirror system, modeled by a time-delay fourth order system, was studied in [76].
- Within a collaboration with *Safran Tech Laboratory* and *Safran Electronics & Defense*, in [98], we propose a symbolic method for the explicit computation of certain invariant observers studied in navigation theory.
- An experimental synchronization of a family of a recently proposed oscillator model (i.e. the Brockett oscillator) was studied and implemented in [12].
- In [13], high frequency measurements of various water characteristics and nutrients information of the Marel-Carnot sea monitoring station (Boulogne-sur-Mer, France) have been used to identify a physiological model for phytoplankton bloom through the fluorescence signal. An auto-regressive-moving-average with exogenous inputs (ARMAX) model is designed and tested based on the dataset. It was demonstrated that the developed dynamical model can be used for estimating the fluorescence level and for predicting the various states of phytoplankton bloom. Thus, the developed model can be used for monitoring phytoplankton biomass in the water which in turn might give information about unbalanced ecosystem or change in water quality.

- The problem of latency reduction in direct human-computer interaction was considered in [50] and formulated as a trajectory prediction problem. The predictor was constructed as a frequency-domain approximation of the non-casual ideal predictor. This approximation can be computed analytically, or obtained as an optimization task. An adaptive modification of the forecasting algorithm was proposed taking into account possible variations in user behavior.
- In [24], 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 and it complements the ISS theory of multistable dynamics for periodic systems. The efficiency of the proposed approach is illustrated via the global analysis of a nonlinear pendulum with constant persistent input.
- Conditions for almost global stability of an operating point of a realistic model of a synchronous generator with constant field current connected to an infinite bus are derived in [38]. The analysis is conducted by employing the recently proposed concept of input-to-state stability (ISS)–Leonov functions, which is an extension of the powerful cell structure principle developed by Leonov and Noldus to the ISS framework. Compared with the original ideas of Leonov and Noldus, the ISS–Leonov approach has the advantage of providing additional robustness guarantees. The efficiency of the derived sufficient conditions is illustrated via numerical experiments. This article is part of the themed issue 'Energy management: flexibility, risk and optimization'.
- Conditions for existence and global attractivity of the equilibria of a realistic model of a synchronous generator with constant field current connected to an infinite bus are derived in [14]. First, necessary and sufficient conditions for existence and uniqueness of equilibrium points are provided. Then, sufficient conditions for local asymptotic stability and almost global attractivity of one of these equilibria are given. The analysis is carried out by employing a new Lyapunov–like function to establish convergence of bounded trajectories, while the latter is proven using the powerful theoretical framework of cell structures pioneered by Leonov and Noldus. The efficiency of the derived sufficient conditions is illustrated via extensive numerical experiments based on two benchmark examples taken from the literature.
- In [96], we propose a new approach for testing the stability of *n*D systems. The standard stability conditions are transformed into algebraic conditions and then checked by means of computer algebra techniques for solving algebraic systems such as Gröbner bases, univariate representations and discriminant varieties. The corresponding results were implemented in Maple.
- In [17], we address the problem of computing stabilizing controllers for a specific class of multidimensional SISO systems. This problem, which was an open problem (i.e., no effective methods were existing for the computation of stabilizing controllers), has been solved using techniques from computer algebra. As a result, an effective test of stabilizability as well as an algorithm for computing stabilizing controllers were developed.
- We have recently proposed a new method for the *anchor position self-calibration problem*, a rather well-known problem in the signal processing community. In essence, given two sets of wireless communicating devices, i.e. sources and sensors lying in the three dimensional space, the self-calibration algorithm estimates the position of the devices by only using the source–sensor distance measurements. We have first reformulated the problem in terms of certain matrix equalities. They can then be studied in detail by means of computer algebra methods such as Gröbner basis techniques and the package OreModules. Coupling symbolic methods with standard linear algebra techniques, we obtain a general solution in all dimensions. In particular, for a space of dimension three, very compact closed-form solutions are obtained in a particular reference frame. Thanks to these closed-form solutions, the noise effect can then be characterized yielding the synthesis of realtime filtering to mitigate the effect of the measurement noise. Finally, the resulting implementation is rather

straightforward and based on real-time operations. Additionally, the underlying numerical tools are standard (least-squares, low-rank factorization, matrix calculus) and well-known. The result of this work is being transferred to a patent. A software prototype AutoCal (https://bil.inria.fr/fr/search/query?terms=AutoCal in the BIL) is available on the server AutoCalibrationserver (https://allgo.inria.fr/webapps/166) under the Inria platform AllGO, which allows the user to test the implemented algorithm on his own dataset.

## **QUANTIC Project-Team**

## 6. New Results

## 6.1. Quantum Walks and accelerated mixing algorithms

Participants: A. Sarlette

This major line of work has been pursued together with S.Apers (UGent) and F.Ticozzi (U.Padova), in an attempt to distinguish what is "necessarily" quantum in such models, and what could be explained by memory effects which we could mimic with just classical dynamic controllers. We hence have a series of papers on both sides (quantum and non-quantum): the conference papers are published, the journal papers will be for 2018.

In [19], we investigate under which conditions a higher-order Markov chain, or more generally a Markov chain on an extended state space, can mix faster than a standard Markov chain on a graph of interest. We find that, depending on the constraints on the dynamics, two very different scenarios can emerge: under strict invariance of the target marginal and for general initialization of the lifted chain no speedup is possible; on the other hand, if these requirements are both relaxed, the lifted dynamics can achieve mixing in a time that corresponds to the diameter of the graph, which is optimal.

In [20], we establish a discrete-geometric bound on the convergence speed of mixing with *any* local stochastic process, under the key assumption that it leaves the target distribution invariant at each time. These processes include classical algorithms, any quantum algorithms, as well as possibly other strategies that obey the non-signalling criterion of probability transmission. We explicitly give the bound in terms of isoperimetric inequalities. We illustrate how this general result leads to new bounds on convergence times beyond the explicit Markovian setting. Mixing is essentially concerned with the discrete-time spreading of a distribution along the edges of a graph. In essence we establish that even by exploiting global information about the graph and allowing a very general use of this information, this spreading can still not be accelerated beyond the so-called *conductance bound*. An upcoming journal paper will discuss which assumption changes do lead to faster algorithms, and argue how relevant they are for practical applications.

In [26], we give a preview on our specific results about Quantum walks. Quantum walks have been linked to acceleration in various information processing tasks, and proposed as a possible model for quantum-enhanced behavior in biological systems. These links and acceleration claims have been made with various levels of detail. Here we consider discrete-time quantum walks, and focus on the task of mixing, i.e., distributing the state over a graph. Previous papers have observed that the so-called coined quantum walks can accelerate mixing on certain graphs with respect to the optimal classical Markov chain. We here show that the same speedup can be attained with a classical process, if a similar classical coin is added. We establish a precise correspondence between the mixing performance of quantum walks and such " lifted walks " for all (finite) graphs, and thereby improve known bounds on quantum walk mixing time. We conclude that the advantage of quantum walks with respect to classical processes is not in the mixing speed of the optimal design. However, a notable quantum advantage might reside in the fact that the mixing speed obtained with suboptimal designs, due to for instance limited graph knowledge, appears to be generically faster. The journal version is being finalized and will be sumbitted before the end of 2017.

## 6.2. String Stability towards Leader thanks to Asymmetric Bidirectional Controller

Participants: A. Sarlette

This result published in [21] is the result of an investigation of classical (non-quantum) distributed and coupled systems and their fundamental limitations – a sequel of A.Sarlette's previous line of work. It deals with the problem of string stability of interconnected systems with double-integrator open loop dynamics (e.g. acceleration-controlled vehicles). We analyze an asymmetric bidirectional linear controller, where each vehicle is coupled solely to its immediate predecessor and to its immediate follower with different gains in these two directions. We show that in this setting, unlike with unidirectional or symmetric bidirectional controllers, string stability can be recovered when disturbances act only on a small (N-independent) set of leading vehicles. This improves existing results from the literature with this assumption. We also indicate that string stability with respect to arbitrarily distributed disturbances cannot be achieved with this controller.

A journal version is in preparation where we essentially close the subject, on a discrete-controller version:

- we will show that no local digital controller whatsoever (including nonlinearity, local communication,...) can achieve the academic property of string stability for infinite length chains and with bounded noise/disturbance on *each* member of the chain, and this implies serious consequences for practical behaviors of finite-length chains.

- conversely, we give the equivalent of the above result to show that if one is concerned mainly about the noise/disturbance acting on the leader (boundary condition of the chain), then indeed our above result achieves all existing variants of the string stability definitions.

## 6.3. Towards generic adiabatic elimination for bipartite open quantum systems

Participants: R. Azouit, A. Sarlette, P. Rouchon (and F. Chittaro, visitor in 2016)

The paper [12] is the main paper summarizing the results of the PhD thesis of R.Azouit. We give a theoretical method, with a directly applicable recipe for the physicists who would want to use it, and with examples worked out on applications that experimentalists (e.g. in the partner group at Yale U.) are actually considering nowadays.

We consider a composite open quantum system consisting of a fast subsystem coupled to a slow one. Using the timescale separation, we develop an adiabatic elimination technique to derive at any order the reduced model describing the slow subsystem. The method, based on an asymptotic expansion and geometric singular perturbation theory, ensures the physical interpretation of the reduced second-order model by giving the reduced dynamics in a Lindblad form and the state reduction in Kraus map form. We give explicit secondorder formulas for Hamiltonian or cascade coupling between the two subsystems. These formulas can be used to engineer, via a careful choice of the fast subsystem, the Hamiltonian and Lindbald operators governing the dissipative dynamics of the slow subsystem.

# 6.4. Deterministic submanifolds and analytic solution of the quantum stochastic differential master equation describing a monitored qubit

Participants: A. Sarlette, P. Rouchon

In the paper [18], we study the stochastic differential equation (SDE) associated with a two-level quantum system (qubit) subject to Hamiltonian evolution as well as unmonitored and monitored decoherence channels. The latter imply a stochastic evolution of the quantum state (density operator), whose associated probability distribution we characterize. We first show that for two sets of typical experimental settings, corresponding either to weak quantum non demolition measurements or to weak fluorescence measurements, the three Bloch coordinates of the qubit remain confined to a deterministically evolving surface or curve inside the Bloch sphere. We explicitly solve the deterministic evolution, and we provide a closed-form expression for the probability distribution on this surface or curve. Then we relate the existence in general of such deterministically evolving submanifolds to an accessibility question of control theory, which can be answered with an explicit algebraic criterion on the SDE. This allows us to show that, for a qubit, the above two sets of weak measurements are essentially the only ones featuring deterministic surfaces or curves.

This paper was motivated by a striking experimental observation of Ph.Campagne-Ibarcq (group of Benjamin Huard - now at ENS Lyon and still collaborator). It appears to be actually quite general, and to generalize to higher-dimensional systems than the qubit. We are working on this extension, time permitting (as we have no student support currently), to publish a complete story about relevant experimental systems where the QSDE can be modeled in a very low-dimensional manifold.

## 6.5. Loss-tolerant parity measurement for distant quantum bits

#### Participants: A. Sarlette, M. Mirrahimi

This work, published in [17], [24], is part of the major line of work led by M.Mirrahimi about stabilizing distant entangled states. The latter are a major building block in quantum information technology, thanks to their ability to enable quantum teleportation. They are supposed to play a major 'quantum-bus-type' role in some of the most promising quantum computing architectures.

In this paper, 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 capability enables deterministic preparation of highly entangled qubit states whose fidelity is not limited by the transmission loss. The key observation is that for a probe electromagnetic field in a particular quantum state, namely a superposition of two coherent states of opposite phases, the transmission loss stochastically applies a near-unitary back-action on the probe state. This leads to a parity measurement protocol where the main effect of the transmission losses is a decrease in the measurement strength. By repeating the non-destructive (weak) parity measurement, one achieves a high-fidelity entanglement in spite of a significant transmission loss.

# 6.6. Discrete-time reservoir engineering with entangled bath and stabilizing squeezed states

#### Participants: Z. Miao and A. Sarlette

The paper [15] is the first result of a line of work that we try to establish about the possible use of "timestructured reservoirs" towards stabilizing more complicated states of quantum systems. In particular, we here analyze a setting where reservoir items (qubits) are entangled over discrete time, and we show how it stabilizes squeezed states of a quantum harmonic oscillator. The parameters of the stabilized state can be tuned at will, in tradeoff with the convergence speed. The squeezing direction is determined by the phase of entanglement, thus allowing to distinguish genuine entanglement from mere classical correlations.

This work has allowed to identify the following lines for future research:

- first check time-varying, non-entangled reservoir inputs: from the same mathematical model, it appears that they can also stabilize squeezed states.

- provide a proof, on a non-trivial setting, of the specific benefit of entangled inputs: i.e. show how they achieve stabilization of some interesting states which are not accessible with any non-entangled inputs.

- laying the premises of possible approaches to studying continuous-time reservoir inputs which are entangled over time. This is currently an open question even from the modeling perspective.

## 6.7. Observing a quantum Maxwell demon at work

Participants: R. Azouit, B. Huard and P. Rouchon

The results of this section were published [14]

In apparent contradiction to the laws of thermodynamics, Maxwell's demon is able to cyclically extract work from a system in contact with a thermal bath exploiting the information about its microstate. The resolution of this paradox required the insight that an intimate relationship exists between information and thermodynamics. Here, this Maxwell demon experiment tracks the state of each constituent both in the classical and quantum regimes. The demon is a microwave cavity that encodes quantum information about a superconducting qubit and converts information into work by powering up a propagating microwave pulse by stimulated emission. Thanks to the high level of control of superconducting circuits, direct measurements (combined with maximum-likelihood estimation techniques inspired by [90]) give the extracted work and entropy remaining in the demon's memory. This experiment provides an enlightening illustration of the interplay of thermodynamics with quantum information.

# 6.8. Asymptotic expansions of Laplace integrals for quantum state tomography

Participant: P. Rouchon (with his former PhD student P. Six)

The results of this section were published in [25].

Bayesian estimation of a mixed quantum state can be approximated via maximum likelihood (MaxLike) estimation when the likelihood function is sharp around its maximum. Such approximations rely on asymptotic expansions of multi-dimensional Laplace integrals. When this maximum is on the boundary of the integration domain, as it is the case when the MaxLike quantum state is not full rank, such expansions are not standard. We provide here such expansions, even when this maximum does not belong to the smooth part of the boundary, as it is the case when the rank deficiency exceeds two. These expansions provide, aside the MaxLike estimate of the quantum state, confidence intervals for any observable. They confirm the formula proposed and used without precise mathematical justifications by the authors in an article published in Physical Review A in 2016 [90].

# 6.9. Generating higher order quantum dissipation from lower order parametric processes

Participant: M. Mirrahimi (and S. Mundhada, visitor from Yale in 2016)

The results of this section were published in [16].

Stabilization of quantum manifolds is at the heart of error-protected quantum information storage and manipulation. Nonlinear driven-dissipative processes achieve such stabilization in a hardware efficient manner. Josephson circuits with parametric pump drives implement these nonlinear interactions. In this work, we propose a scheme to engineer a four-photon drive and dissipation on a harmonic oscillator by cascading experimentally demonstrated two-photon processes. This would stabilize a four-dimensional degenerate manifold in a superconducting resonator. We analyze the performance of the scheme using numerical simulations of a realizable system with experimentally achievable parameters. This theoretical work, initiated by Shantanu Mundhada during his visit to Inria in 2016, is currently investigated experimentally at Yale.

# 6.10. Degeneracy-preserving quantum nondemolition measurement of parity-type observables for cat qubits

Participant: J. Cohen, M. Mirrahimi

The results of this section were published in [13] and correspond to an important chapter of J. Cohen's thesis [11].

A central requirement for any quantum error correction scheme is the ability to perform quantum nondemolition measurements of an error syndrome, corresponding to a special symmetry property of the encoding scheme. It is in particular important that such a measurement does not introduce extra error mechanisms, not included in the error model of the correction scheme. In this work, we ensure such a robustness by designing an interaction with a measurement device that preserves the degeneracy of the measured observable. More precisely, we propose a scheme to perform continuous and quantum nondemolition measurement of photonnumber parity in a microwave cavity. This corresponds to the error syndrome in a class of error correcting codes called the cat codes, which have recently proven to be efficient and versatile for quantum information processing. In our design, we exploit the strongly nonlinear Hamiltonian of a high-impedance Josephson circuit, coupling a high-Q storage cavity mode to a low-Q readout one. By driving the readout resonator at its resonance, the phase of the reflected or transmitted signal carries directly exploitable information on paritytype observables for encoded cat qubits of the high-Q mode. This important result has defined a new line of experimental research persued by the experimentalists of the Quantic team and Yale university.

## **SPHINX Project-Team**

## 7. New Results

## 7.1. Control and stabilization of heterogeneous systems

## 7.1.1. Analysis of heterogeneous systems

Participants: Jean-François Scheid, Takéo Takahashi.

In [12], we consider a single disk moving under the influence of a 2D viscous fluid and study the asymptotic as the size of the solid tends to zero. If the density of the solid is independent of the size, the energy equality is not sufficient to obtain a uniform estimate for the solid velocity. This is 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.

In [10], we propose a new model for the motion of a viscous incompressible fluid. More precisely, we consider the Navier-Stokes system with a boundary condition governed by the Coulomb friction law. With this boundary condition, the fluid can slip on the boundary if the tangential component of the stress tensor is too large. We prove the existence and uniqueness of a weak solution in the two-dimensional problem and the existence of at least one solution in the three-dimensional case. In [9], we consider this model with a rigid body. We prove that there exists a weak solution for the corresponding system.

In [13], we study 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's law. We prove the existence and uniqueness of global in time strong solutions. The main novelty is that we include the case of non homogeneous boundary conditions.

In [31], we study the shape differentiability of the free-boundary 1-dimensional simplified model for a fluidelasticity system. The full characterization of the associated material derivatives is given and the shape derivative of an energy functional has been obtained.

#### 7.1.2. Control of heterogeneous systems

Participants: Thomas Chambrion, Alessandro Duca, Takéo Takahashi.

In [11], we consider the swimming into a stationary Navier-Stokes fluid. The swimmer is a rigid body  $S \subset \mathbb{R}^3$  immersed in an infinitely extended fluid. We are interested in self-propelled motions of S in the steady state regime of the rigid body-fluid system, assuming that the mechanism used by the body to reach such a motion is modeled through a distribution of velocities on the boundary. We show that this can be solved as a control problem.

In [16] we prove that the Kuramoto-Sivashinsky equation is locally controllable in 1D and in 2D with one boundary control. His method consists in combining several general results in order to reduce the null-controllability of this nonlinear parabolic equation to the exact controllability of a linear beam or plate system. This improves known results on the controllability of Kuramoto-Sivashinsky equation and gives a general strategy to handle the null-controllability of nonlinear parabolic systems.

The paper [21] is the result of a long term analysis about the restrictions to the controllability of bilinear systems induced by the regularity of the propagators for the bilinear Schrödinger equation. This paper comes along with its companion paper [20] which gives a detailed proof of the celebrated Ball-Marsden-Slemrod obstruction to exact controllability for bilinear systems with  $L^1$  controls.

The paper [23] is concerned with the one dimensional bilinear Schrödinger equation in a bounded domain. In this article, we have given the first available upper bound estimates of the time needed to steer exactly the infinite square potential well from its first eigenstate to the second one.

In [22], we present an embedded automatic strategy for the control of a low consumption vehicle equipped with an "on/off" engine. The proposed strategy has been successfully implemented on the Vir'Volt prototype in official competition (European Shell Eco Marathon).

## 7.1.3. Stabilization of heterogeneous systems

Participants: David Dos Santos Ferreira, Takéo Takahashi, Julie Valein, Jean-Claude Vivalda.

In [8], we find, thanks to a a semiclassical approach,  $L^p$  estimates for the resolvants of the damped wave operator given on compact manifolds whose dimension is greater than 2.

In [7], we study the feedback stabilization of a system composed by an incompressible viscous fluid and a deformable structure located at the boundary of the fluid domain. We stabilize the position and the velocity of the structure and the velocity of the fluid around a stationary state by means of a Dirichlet control, localized on the exterior boundary of the fluid domain and with values in a finite dimensional space.

In [19], we study the nonlinear Korteweg-de Vries equation with boundary time-delay feedback. Under appropriate assumption on the coefficients of the feedbacks, we first prove that this nonlinear infinite dimensional system is well-posed for small initial data. The main results of our study are two theorems stating the exponential stability of the nonlinear time delay system, using two different methods: a Lyapunov functional approach and an observability inequality approach.

In [14], we generalize a formula, due to E. Sontag *et al.*, giving explicitly a continuous stabilizing feedback for systems affine in the control; more specifically for a large class of systems which depend quadratically on the control, an explicit formula for a stabilizing feedback law is given.

## 7.2. Inverse problems for heterogeneous systems

#### 7.2.1. Reconstruction of coefficients and initial conditions

Participants: Karim Ramdani, Julie Valein, Jean-Claude Vivalda.

In [79], we proposed an algorithm for estimating from partial measurements the population for a linear agestructured population diffusion model. In this work, the physical parameters of the model were assumed to be known. In [29], we investigate the inverse problem of simultaneously estimating the population and the spatial diffusion coefficient for an age-structured population model. The measurement used is the time evolution of the population on a subdomain in space and age. The proposed method is based on the generalization to the infinite dimensional setting of an adaptive observer originally proposed for finite dimensional systems.

In [18], we show that, generically, a (finite dimensional) sampled system is observable provided that the number of outputs is at least equal to the number of inputs plus 2. This work complements some previous works on the subject.

### 7.2.2. Geometrical inverse problems

Participants: Alexandre Munnier, Karim Ramdani, Takéo Takahashi.

In [75], we proposed an explicit reconstruction formula for a two-dimensional cavity inverse problem. The proposed method was limited to the case of a single cavity due to the use of conformal mappings. In [28], we consider the case of a finite number of cavities and aim to recover the location and the shape of the cavities from the knowledge of the Dirichlet-to-Neumann (DtN) map of the problem. The proposed reconstruction method is non iterative and uses two main ingredients. First, the authors show how to compute so-called generalized Pólia-Szegö tensors (GPST) of the cavities from the DtN of the cavities. Secondly, the authors shows that the obtained shape from GPST inverse problem can be transformed into a shape from moments problem, for some particular configurations. However, numerical results suggest that the reconstruction method is efficient for arbitrary geometries.

In [15], we consider the geometrical inverse problem consisting in recovering an unknown obstacle in a viscous incompressible fluid by measurements of the Cauchy force on the exterior boundary. We deal with the case where the fluid equations are the nonstationary Stokes system and using the enclosure method, we can recover the convex hull of the obstacle and the distance from a point to the obstacle. With the same method, we can obtain the same result in the case of a linear fluid-structure system composed by a rigid body and a viscous incompressible fluid.

## 7.3. Numerical analysis and simulation of heterogeneous systems

Participants: Xavier Antoine, Qinglin Tang.

In [1], we propose a simple accelerated pseudo-spectral algorithm to compute the stationary states of the Gross-Piteavskii Equation (GPE) with possibly multiple components. The method is based on the adaptation of new optimization algorithms under constraints coming from mathematical imaging to the imaginary time (gradient-like) method for the GPE arising in Bose-Einstein Condensation.

In [3] we propose original efficient preconditioned conjugate gradient methods coming from molecular physics to the GPE for spectrally computing the stationary states of the GPE. The method allows a gain of a factor 100 for 3D problems with extremely large nonlinearities and fast rotations. The HPC solver is being developed.

In [17], we develop new robust and efficient algorithms for computing the dynamics of 2-components GPEs with dipolar interaction. The main particularity of the method is that high accuracy is obtained by a new FFT based evaluation of nonlocal kernels applied to the nonlinear part of the operator.

In [4], we propose an asymptotic mathematical analysis of domain decomposition techniques for solving the 1D nonlinear Schrödinger equation and GPE. The analysis uses advanced techniques related to fractional microlocal analysis for PDEs. Simulations confirm the mathematical analysis.

In [2], we extend, by some very technical mathematical analysis, approaches for the results stated in [4]. Again, numerical simulations validate the theoretical analysis.

In [5], we develop and implement in parallel simple new solvers for computing the dynamics of solutions to the Dirac equation arising in quantum physics. Numerical examples are developed to analyze the capacity of these algorithms for a parallel implementation.

In [6], we introduce the concept of Absorbing Boundary Conditions and Perfectly Matched Layers for the dynamics of nonlinear problems related to classical and relativistic quantum wave problems (Wave equation, Schrödinger equation, Dirac equation). In particular, we show application examples and detail the methods so that they can be implemented by researchers coming for quantum physics.

## **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.

The PhD work of Antoine Hochart [88] was dealing 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 [52] for the case of bounded paiements. A more general approach was developed in [87], 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. A more recent work include the introduction of an abstract game allowing us to deal with general monotone additively homogeneous operators and thus to unbounded paiements.

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 [12].

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 [13]. This extends to the two-player case known representation theorems for risk measures.

#### 7.1.2. The operator approach to entropy games

Participants: Marianne Akian, Stéphane Gaubert.

Entropy games were recently introduced by Asarin et al. A player (Despot) wishes to minimize a measure of "freedom" given by a topological entropy, whereas the other player (Tribune) wishes to maximize it. In [25], we developed an operator approach for entropy games. We showed that they reduce to risk sensitive type game problems, and deduced that entropy games in Despot has a few positions with non-trivial actions can be solved in polynomial time.

## 7.1.3. 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.

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. In [47], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [91], [97] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [74] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [38], [39] (also presented in [24]), we improve the method of Fahim, Touzi and Warin by introducing probabilistic schemes which are monotone without any restrictive condition, allowing one to solve fully nonlinear parabolic partial differential equations. We study the convergence and obtain error estimates when the parameters and the value function are bounded. We are now studying the more general quadratic growth case.

## 7.1.4. Tropical-SDDP algorithms for stochastic control problems involving a switching control

Participants: Marianne Akian, Duy Nghi, Benoît Tran.

The PhD thesis of Benoît Tran, supervised by Jean-Philippe Chancelier (ENPC) and Marianne Akian concerns the numerical solution of the dynamic programming equation of discrete time stochastic control problems.

Several methods have been proposed in the litterature to bypass the curse of dimensionality difficulty of such an equation, by assuming a certain structure of the problem. Examples are the max-plus based method of McEneaney [98], [99], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [104], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [60], the probabilistic numerical method of Fahim, Touzi and Warin [74]. We propose to associate and compare these methods in order to solve more general structures, in particular problems involving a finite set-valued (or switching) control and a continuum-valued control, with the property that the value function associated to a fixed switching strategy is convex.

# 7.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

## 7.2.1. Order reversing maps on cones

Participant: Cormac Walsh.

We have been studying non-linear operators on open cones, particularly ones that preserve or reverse the order structure associated to the cone. A bijective map that preserves the order in both directions is called an order isomorphism. Those that reverse the order in both directions are order antimorphisms. These are closely related to the isometries of the Hilbert and Thompson metrics on the cone.

Previously, we have shown [118] that if there exists an antimorphism on an open cone that is homogeneous of degree -1, then the cone must be a symmetric cone, that is, have a transitive group of linear automorphisms and be self-dual.

The technique was to consider the Funk metric on the cone, which is a non-symmetric metric defined using the order and homogeneity structures. Each antimorphism on a cone that is homogeneous of degree -1 reverses this metric, and so interchanges the two horofunction boundaries of the metric, the one in the forward direction and the one in the backward direction. By studying these boundaries we obtained the result.

More recently, we have shown [45] that the homogeneity assumption is not actually necessary: every antimorphism on a cone is automatically homogeneous of degree -1.

Without the homogeneity assumption, the metric techniques do not work. Instead, it was necessary to study how the map acts on line segments parallel to extreme rays of the cone. This is similar to the what was done by Rothaus, Noll and Schäffer, and Artstein-Avidan and Slomka in their work on order isomorphisms. This means that our proof is essentially finite dimensional. Indeed, there are many interesting cones in infinite dimension that have few or no extreme rays. In infinite dimension, it is natural to consider order unit spaces as a generalisation of cones, and JB-algebras as a generalisation of symmetric cones. Lemmens, Roelands, and Wortel have asked whether the existence of an order antimorphism that is homogeneous of degree -1 on the cone of an order-unit space implies that the space is a JB-algebra? The result above suggests further that one might even be able to drop the homogeneity assumption.

## 7.2.2. 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 [115], we refined this theorem by characterizing the set of minimal upper bounds: we showed that it is homeomorphic to the quotient space  $O(p) \\ O(p,q)/O(q)$ , where O(p,q) denotes the orthogonal group associated to the quadratic form with signature (p,q), and O(p) denotes the standard *p*th orthogonal group.

## 7.2.3. 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 [20], 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].

In [27], we have made the first steps of a formalization of the theory of convex polyhedra in the proof assistant Coq. The originality of our approach lies in the fact that our formalization is carried out in an effective way, in the sense that the basic predicates over polyhedra (emptiness, boundedness, membership, etc) are defined by means of Coq programs. All these predicates are then proven to correspond to the usual logical statements. The latter take the form of the existence of certificates: for instance, the emptiness of a polyhedron is shown to be equivalent to the existence of a certificate *a la* Farkas. This equivalence between Boolean predicates and formulas living in the kind Prop is implemented by using the boolean reflection methodology, and the effective nature of our approach is demonstrated by the fact that we easily arrive at the proof of important results on polyhedra, such as several versions of Farkas Lemma, duality theorem of linear programming, separation from convex hulls, Minkowski Theorem, etc.

Our effective approach is made possible by implementing the simplex method inside Coq, and proving its correctness and termination. Two difficulties need to be overcome to formalize it. On the one hand, we need to deal with its termination. More precisely, the simplex method iterates over the so-called bases. Its termination depends on the specification of a pivoting rule, whose aim is to determine, at each iteration, the next basis. In this work, we have focused on proving that the lexicographic rule ensures termination. On the other hand, the simplex method is actually composed of two parts. The part that we previously described, called Phase II, requires an initial basis to start with. Finding such a basis is the purpose of Phase I. It consists in building an extended problem (having a trivial initial basis), and applying to it Phase II. Both phases need to be formalized to obtain a fully functional algorithm. a

## 7.3.2. Tropical totally positive matrices

Participant: Stéphane Gaubert.

In [81] (joint work with Adi Niv) we investigate the tropical analogues of totally positive and totally nonnegative matrices, i.e, the images by the valuation of the corresponding classes of matrices over a nonarchimedean field. We show in particular that tropical totally positive matrices essentially coincide with the Monge matrices (defined by the positivity of  $2 \times 2$  tropical minors), arising in optimal transport. More recent developments include relations between tropical total positivity and planar networks.

#### 7.3.3. Tropical compound matrix identities

Participants: Marianne Akian, Stéphane Gaubert.

A number of polynomial identities in tropical semirings can be derived from their classical analogues by application of a transfer principle [49], [51]. In the present work [40], joint with Adi Niv, we prove identities on compound matrices in extended tropical semirings, which cannot be obtained by transfer principles, but are rather obtained by combinatorial methods. Such identities include analogues to properties of conjugate matrices, powers of matrices and 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.

## 7.3.4. Group algebra in characteristic one and invariant distances over finite groups Participant: Stéphane Gaubert.

In [19] (joint work with Dominique Castella), we investigated a tropical analogue of group algebras. We studied tropical characters and related them to invariant distances over groups.

### 7.3.5. Volume and integer points of tropical polytopes

Participants: Marie Maccaig, Stéphane Gaubert.

We investigate in [43] 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  $2^{\text{poly}(m,n)}$  existing unless P = NP. We further proved the  $\sharp P$ -hardness for the analogous problems for tropical polytopes instead defined by inequalities.

# 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.

In [14], with Meisam Sharify (IPM, Tehran, Iran), we 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 [46].

## 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 (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  $(x^{\mu}, w^{\mu})$  of the barrier problems:

minimize 
$$c \cdot x - \mu(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i)$$
  
subject to  $Ax + w = b, \ x > 0, \ w > 0$ 

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 Smale 9th problem [113], 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 [71], [70], [73], [72]. In particular, by analogy with the classical Hirsch conjecture, Deza, Terlaky and Zinchencko [72] proposed the "continuous analogue of the Hirsch conjecture", which says that the total curvature of the central path is linearly bounded in the number m of constraints.

In a work of X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig [41], we prove that primal-dual logbarrier interior point methods are not strongly polynomial, by constructing a family of linear programs with 3r + 1 inequalities in dimension 2r for which the number of iterations performed is in  $\Omega(2^r)$ . The total curvature of the central path of these linear programs is also exponential in r, disproving the continuous analogue of the Hirsch conjecture.

Our method is to tropicalize the central path in linear programming. The tropical central path is the piecewiselinear limit of the central paths of parameterized families of classical linear programs viewed through logarithmic glasses. We give an explicit geometric characterization of the tropical central path, as a tropical analogue of the barycenter of a sublevel set of the feasible set induced by the duality gap. We study the convergence properties of the classical central path to the tropical one. This allows us to show that that the number of iterations performed by interior point methods is bounded from below by the number of tropical segments constituting the tropical central path.

### 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

$$\left\{ x \in \mathbb{R}^n : Q^{(0)} + x_1 Q^{(1)} + \dots + x_n Q^{(n)} \succeq 0 \right\}$$

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  $NP_{\mathbb{R}} \cap coNP_{\mathbb{R}}$ , 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 [59].

Then, we show in [17] 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 NP  $\cap$  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.

A long-standing problem is to characterize the convex semialgebraic sets that are SDP representable, meaning that they can be represented as the image of a spectrahedron by a (linear) projector. Helton and Nie conjectured that every convex semialgebraic set over the field of real numbers are SDP representable. Recently, [110] disproved this conjecture. In [26], we show, however, that the following result, which may be thought of as a tropical analogue of this conjecture, is true: over a real closed nonarchimedean field of Puiseux series, the convex semialgebraic sets and the projections of spectrahedra have precisely the same images by the nonarchimedean valuation. The proof relies on game theory methods applied to our previous results [59] and [17].

## 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 section presents the PhD work of Nikolas Stott. An essential part of the present work is in collaboration with Éric Goubault and Sylvie Putot (from LIX).

We develop a 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 7.2.2).

The initial part of this work was described in the article [57], in which we obtained a single ellipsoidal invariant. In [16], we showed that finer disjunctive invariants, expressed as union of ellipsoids, can still be obtained by nonlinear fixed point methods in a scalable way. In [30], we developed a dual approach, which we applied to the problem of computing the joint spectral radius. We showed that an approximation of a Barabanov norm by a supremum of quadratic forms can be obtained by solving a nonlinear eigenvalue problem involving "tropical Kraus maps". The latter can be thought of as the tropical analogues of the completely positive maps appearing in quantum information. The fixed point methods in [30] allow one to solve large scale instances, unaccessible by earlier (LMI based) methods.

#### 7.5.2. Performance evaluation of an emergency call center

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), now with PP. 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.

We initially introduced a discrete model in [54], 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. We showed 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. However, the convergence to a stationary regime may not occur in the discrete model. We developed in [15] a continuous time analogue of this model, involving a piecewise linear dynamical systems, and showed that it has the same stationary regimes, avoiding some pathologies of the discrete model.

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. This analysis has been recovered by a probabilistic model in [42].

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 combined explicit analytic computations of the different congestion phases of a simplified model and extensive simulations of a realistic an detailed model, to evaluate the performance of the center as a function of the number of operators. This analysis also suggested some ways to monitor early signs of potential congestions as well as possible correcting measures to avoid congestion.

### 7.5.3. Tropical models of fire propagation in urban areas

Participants: Stéphane Gaubert, Daniel Jones.

As part of the team work in the ANR project Democrite, we developed a model of fire propagation in urban areas, involving a discrete analogue of a Hamilton-Jacobi PDE. This models indicates that the fire propagates according to polyhedral ball, which is in accordance from data from historical fires (London, Chicago, or more recently Kobe).

#### 7.5.4. 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 is presented in [28]. In a followup work (collaboration with Gleb Koshevoy), we managed to extend these results to wider classes of bilevel problems, and to relate them to competitive equilibria problems.

## 7.5.5. Game theory models of decentralized mechanisms of pricing of the smart grid

Participants: Stéphane Gaubert, Paulin Jacquot.

This work is in collaboration with Nadia Oudjane and Olivier Beaude (EDF).

The PhD work of Paulin Jacquot concerns the application of game theory techniques to pricing of energy. We are developing a game theory framework for demand side management in the smart grid, in which users have movable demands (like charging an electric vehicle). We compared in particular the daily and hourly billing mechanisms. The latter, albeit more complex to analyse, has a merit in terms of incitatives, as it leads the user to move his or her consumption at off peak hours. We showed the Nash equilibrium is unique, under some assumptions, and gave theoretical bounds of the price of anarchy of the game with a hourly billing, showing this mechanism remains efficient while being more "fair" than the daily billing. We proposed and tested decentralized algorithms to compute the Nash equilibrium. These contriutions are presented In [31], [32], [44].

## **DOLPHIN Team**

## 7. New Results

## 7.1. Fitness Landscape Analysis for Algorithm Understanding, Selection, Design and Configuration

Participants: Bilel Derbel, Arnaud Liefooghe (external collaborators: Sebastien Verel, Univ. Littoral, France; Hernan Aguirre, Fabio Daolio, Hugo Monzón, Miyako Sagawa and Kiyoshi Tanaka, Shinshu University, Japan)

**Fitness landscape analysis of Pareto local search on bi-objective permutation flowshop scheduling problems.** In [20], we study the difficulty of solving different bi-objective formulations of the permutation flowshop scheduling problem by adopting a fitness landscape analysis perspective. Our main goal is to shed the light on how different problem features can impact the performance of Pareto local search algorithms. Specifically, we conduct an empirical analysis addressing the challenging question of quantifying the individual effect and the joint impact of different problem features on the success rate of the considered approaches. Our findings support that multi-objective fitness landscapes enable to devise sound general-purpose features for assessing the expected difficulty in solving permutation flowshop scheduling problems, hence pushing a step towards a better understanding of the challenges that multi-objective randomized search heuristics have to face.

Landscape-aware automatic algorithm configuration. The proper setting of algorithm parameters is a well-known issue that gave rise to recent research investigations from the (offline) automatic algorithm configuration perspective. Besides, the characteristics of the target optimization problem is also a key aspect to elicit the behavior of a dedicated algorithm, and as often considered from a landscape analysis perspective. In [21], we show that fitness landscape analysis can open a whole set of new research opportunities for increasing the effectiveness of existing automatic algorithm configuration methods. Specifically, we show that using landscape features in iterated racing both (i) at the training phase, to compute multiple elite configuration to use on a feature basis, provides significantly better results compared against the standard landscape-oblivious approach. Our first experimental investigations on NK-landscapes, considered as a benchmark family having controllable features in terms of ruggedness and neutrality, and tackled using a memetic algorithm with tunable population size and variation operators, show that a landscape-aware approach is a viable alternative to handle the heterogeneity of (black-box) combinatorial optimization problems.

Learning variable importance to guide recombination on many-objective optimization. There are numerous many-objective real-world problems in various application domains for which it is difficult or timeconsuming to derive Pareto optimal solutions. In an evolutionary algorithm, variation operators such as recombination and mutation are extremely important to obtain an effective solution search. In [25], we study a machine learning-enhanced recombination that incorporates an intelligent variable selection method. The method is based on the importance of variables with respect to convergence to the Pareto front. We verify the performance of the enhanced recombination on benchmark test problems with three or more objectives using the many-objective evolutionary algorithm  $A\epsilon S\epsilon H$  as a baseline algorithm. Results show that variable importance can enhance the performance of many-objective evolutionary algorithms.

**Closed state model for understanding the dynamics of multi-objective evolutionary algorithms.** In [22], we propose the use of simple closed state models to capture, analyze and compare the dynamics of multiand many-objective evolutionary algorithms. Two- and three-state models representing the composition of the instantaneous population are described and learned for representatives of the major approaches to multiobjective optimization, i.e. dominance, extensions of dominance, decomposition, and indicator algorithms. The model parameters are trained from data obtained running the algorithms with various population sizes on enumerable MNK-landscapes with 3, 4, 5 and 6 objectives. We show ways to interpret and use the model
parameter values in order to analyze the population dynamics according to selected features. For example, we are interested in knowing how parameter values change for a given population size with the increase of the number of objectives. We also show a graphical representation capturing in one graph how the parameters magnitude and sign relate to the connections between states.

## 7.2. Multi-objective Demand side management in smart grids

Participants: El-Ghazali Talbi (externel collaborators: Rachid Ellaia, Zineb Garroussi - Univ. Rabat Morocco)

Residential demand side management (DSM) is one of the most challenging topics in smart grids. In this work, a multi-objective model for the residential DSM is proposed. The smart home is composed of appliances, a battery and a photovoltaic panel. The resolution of this model is a matheuristic based on combining a multi-objective evolutionary algorithm and an exact liner programming solver (CPLEX). Candidate solutions in this hybrid approach are incompletely represented in the representation, and the exact solver is used as a decoder to determine the missing parts in an optimal way. In our case, hybridization involves solving a MILP sub-problem by CPLEX to manage the battery and the photovoltaic panel constraints. Through case studies, It is shown that the coordination between the photovoltaic panel and the battery is effective to reduce the total electricity cost, the discomfort and the standard deviation of power consumed especially in summer conditions [17][18].

## 7.3. Fractal based-decomposition optimization algorithm

Participants: El-Ghazali Talbi (externel collaborators: Amir Nakib - Univ. Paris 12 France)

In this work a new metaheuristic based on geometric fractal decomposition to solve large-scale continuous optimization problems is proposed. It consists of dividing the feasible search space into sub-regions with the same geometrical pattern. At each iteration, the most promising ones are selected and further decomposed. This approach tends to provide a dense set of samples and has interesting theoretical convergence properties. Under some assumptions, this approach covers all the search space only in case of small dimensionality problems. The aim of this work is to propose a new algorithm based on this approach with low complexity and which performs well in case of large-scale problems. To do so, a low complex method that profits from fractals properties is proposed. Then, a deterministic optimization procedure is proposed using a single solution-based metaheuristic which is exposed to illustrate the performance of this strategy. Obtained results on common test functions were compared to those of algorithms from the literature and proved the efficiency of the proposed algorithm [8].

## 7.4. Parallel High-Level Search Heuristics for Single- and Multi-objective Optimization

Participants: Bilel Derbel, Arnaud Liefooghe (external collaborators: Sebastien Verel, Univ. Littoral, France; Jialong Shi and Qingfu Zhang, City University, Hong Kong)

A parallel tabu search for the unconstrained binary quadratic programming problem. Although several sequential heuristics have been proposed for dealing with the Unconstrained Binary Quadratic Programming (UBQP), very little effort has been made for designing parallel algorithms for the UBQP. In [26], we propose a novel decentralized parallel search algorithm, called Parallel Elite Biased Tabu Search (PEBTS). It is based on D2TS, a state-of-the-art sequential UBQP metaheuristic. The key strategies in the PEBTS algorithm include: (i) a lazy distributed cooperation procedure to maintain diversity among different search processes and (ii) finely tuned bit-flip operators which can help the search escape local optima efficiently. Our experiments on the Tianhe-2 supercomputer with up to 24 computing cores show the accuracy of the efficiency of PEBTS compared with a straightforward parallel algorithm running multiple independent and non-cooperating D2TS processes.

**Decomposition-based parallel strategies to speed up Pareto local search.** Pareto Local Search (PLS) is a basic building block in many state-of-the-art multiobjective combinatorial optimization algorithms. However, the basic PLS requires a long time to find high-quality solutions. In [27], we propose and investigate several parallel strategies to speed up PLS using decomposition. These strategies are based on a parallel multi-search framework. In our experiments, we investigate the performances of different parallel variants of PLS on the multiobjective unconstrained binary quadratic programming problem. Each PLS variant is a combination of the proposed parallel strategies. The experimental results show that the proposed approaches can significantly speed up PLS while maintaining about the same solution quality. In addition, we introduce a new way to visualize the search process of PLS on two-objective problems, which is helpful to understand the behaviors of PLS algorithms.

### 7.5. Large scale GPU-centric optimization

### Participants: J. Gmys, M. Gobert and N. Melab

This contribution is a joint work with M. Mezmaz 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. N. Melab and M. Mezmaz have been the guest editors [7] of a special issue in the CCPE journal on this topic.

Nowadays, accelerator-centric architectures offer orders-of-magnitude performance and energy improvements. The interest of those parallel resources has been recently accentuated by the advent of deep learning making them definitely key-building blocks of modern supercomputers. During the year 2017, the focus has been put on the investigation of these specific devices within the context of parallel optimization. In the following, two major contributions are reported: (1) massively parallel GPU-centric tree-based optimization for solving to optimality big permutation optimization problems; (2) Cuda Dynamic Parallelism (CDP) for backtracking. Another contribution [2] on the parallel solving of permutation (flow-shop) problems is proposed but not presented here.

- Massively parallel GPU-centric tree-based optimization. Within the context of the Ph.D thesis (jointly supervised with UMONS, Belgium) of Jan Gmys [1], parallel Branch-and-Bound (B&B) has been revisited for multi-core processors, (multi-)GPU accelerators and MIC coprocessors [6]. During the 2017 year, the focus was put on the extension of these contributions in order to deal with large hybrid clusters. A bi-level parallel approach is actually proposed to revisit the parallel B&B at the intra- and inter-processing node levels. The intra-node level consists in the combination of the previous contributions for an efficient exploitation of the parallelism levels provided inside a processing node which can be a multi-core processor, a GPU, a Xeon Phi or their combination (hybrid processing node). The inter-node (cluster) level deals with the parallelism provided through the use of multiple processing nodes. In the PhD thesis of M. Mezmaz, we have investigated such parallelism by proposing a grid-enabled approach called B&B@Grid, including interval-based work stealing (WS) and checkpointing mechanisms. In addition, each processing node is mainly composed of a single processing core processing a single interval at a time. Our contribution consists in revisiting those mechanisms to deal with multi- and many-core resources. Indeed, for instance a GPU explores thousands of intervals. The contribution includes a bi-level WS mechanism together with a multi-interval checkpointing mechanism. The proposed approach has been experimented on the OUESSANT GPU cluster located at IDRIS, Paris. The results show that, on the road to the exascale era, our approach scales up to 130.000 Cuda cores, reducing the execution time from 25 days (using B&B@Grid) to 9 hours.
- Cuda Dynamic Parallelism (CDP) for backtracking. New GPGPU technologies, such as CUDA Dynamic Parallelism (CDP), can help dealing with recursive patterns of computation, such as divideand-conquer, used by backtracking algorithms. During 2017, in collaboration with University of Cearà (Brazil), we have investigated the CDP mechanism using highly irregular algorithms. Indeed, we have proposed a GPU-accelerated backtracking algorithm using CDP that extending a wellknown parallel backtracking model. The algorithm analyzes the memory requirements of subsequent kernel generations and performs no dynamic memory allocation on GPU, unlike related works from the literature. The proposed algorithm has been extensively experimented using the N-Queens Puzzle

problem and instances of the Asymmetric Traveling Salesman Problem (ATSP) as test-cases. The proposed CDP algorithm may, under some conditions, outperform its non-CDP counterpart by a factor up to 25. Compared to other CDP-based strategies from the literature, the proposed algorithm is on average  $8 \times$  faster.

## **GEOSTAT Project-Team**

# 7. New Results

# 7.1. Multifractal desynchronization of the cardiac excitable cell network during atrial fibrillation

### Participants: G. Attuel, H. Yahia.

We compute the so-called multifractal spectra using two variants of the wavelet transform modulus maxima method, the moment (partition function) method and the magnitude cumulant method. Application of these methods to long time series recorded in a patient with chronic AF provides quantitative evidence of the multifractal intermittent nature of the electric energy of passing cardiac impulses at low frequencies, i.e. for times (> 0.5s) longer than the mean interbeat. We also report the results of a two-point magnitude correlation analysis which infers the absence of a multiplicative time-scale structure underlying multifractal scaling. The electric energy dynamics looks like a "multifractal white noise" with quadratic (log-normal) multifractal spectra. These observations challenge concepts of functional reentrant circuits in mechanistic theories of AF, still leaving open the role of the autonomic nervous system (ANS). A transition is indeed observed in the computed multifractal spectra which group according to two distinct areas, consistently with the anatomical substrate binding to the CS, namely the left atrial posterior wall, and the ligament of Marshall which is innervated by the ANS. In a companion paper (II. Modeling), we propose a mathematical model of a denervated heart where the kinetics of gap junction conductance alone induces a desynchronization of the myocardial excitable cells, accounting for the multifractal spectra found experimentally in the left atrial posterior wall area.

Publication: G. Attuel *et al.*, Multifractal desynchronization of the cardiac excitable cell network during atrial fibrillation. I. Multifractal analysis of clinical data. Accepted in **Frontiers in Physiology**, publication beginning 2018.

## 7.2. Super-resolution

Participant: N. Brodu.

N. Brodu, "Super-Resolving Multiresolution Images With Band-Independent Geometry of Multispectral Pixels". IEEE Transactions on Geoscience and Remote Sensing 55(8), p4610-4617, 2017. In this work we introduce a new method to enhance Sentinel-2 images. Sentinel is a leading ESA program in satellite-based environmental monitoring. N. Brodu has included a super-resolution algorithm in the form of a plug-in in the ESA SNAP software. SNAP is a major reference in satellite image processing. Free software (Cecill-C and GPL), APP deposit under way, https://bil.inria.fr/fr/software/view/2984/tab. Publication: [15].

### 7.3. Surface mixing and biological activity in the Northwest African upwelling

Participants: A. El Aouni, K. Daoudi, H. Yahia.

The aim of this work is to study the horizontal stirring and mixing in different upwelling areas of the Northwest African margin using attracting/repelling Lagrangian coherent structures (LCS) obtained as subsets of hyperstreamline of the Cauchy-Green strain tensor, whose normal repulsion rate is larger than tangential stretch over backward/forward time interval, and their link to the chlorophyll fronts concentrations, based on 10 years satellite data. The temporal variability of surface stirring is compared to the fronts chlorophyll concentration. Two of the four studied areas exhibit negative correlation between mixing and the chlorophyll concentration. The other two regions show similar seasonal variations, nearly coincident maxima and minima, leading to a global positive correlation. These results are compared to other works that make use of Finite Size Lyapunov Exponent (FSLE) whose output is a plot of scalar distributions. Furthermore, we compare the chlorophyll concentrations with both compressing and stretching lines. Results show different regions with different properties. The surface mixing and chlorophyll concentrations is governed by stretching lines in two regions, by compressing lines in one region with, while no different is shown between attracting and repelling LCS in the northenrn region of the studied area.

### 7.4. Spatio-Temporal Dynamics of Floods

#### Participant: N. Brodu.

The floods are an annual phenomenon on the Pacific Coast of Ecuador and can become devastating during El Niño years, especially in the Guayas watershed (32,300 km<sup>2</sup>), the largest drainage basin of the South American western side of the Andes. As limited information on flood extent in this basin is available, this study presents a monitoring of the spatio-temporal dynamics of floods in the Guayas Basin, between 2005 and 2008, using a change detection method applied to ENVISAT ASAR Global Monitoring SAR images acquired at a spatial resolution of 1 km.

Publication: [16].

### 7.5. Effect of wind stress forcing on ocean dynamics at Air-Sea Interface

Participant: H. Yahia.

At first order, oceanic currents are generated by the balance of Coriolis and pressure gradient (geostrophic current) and the balance of Coriolis and the frictional force dominated by wind stress in the surface ocean (Ekman current). We aim at studying the difference in term of turbulent hydrodynamics carried by the wind forcing at the air-sea interface. We explore the statistical properties of singularity spectra computed from velocity norms and vorticity data, notably in relation with kurtosis information to underline differences in the turbulent regimes associated with both kinds of velocity fields. This study is conducted over 1 year of daily data and demonstrates the differences in terms of turbulent property of wind forcing. Publication: [24].

## 7.6. Ocean dynamics: frontal activity

#### Participant: H. Yahia.

A highresolution (1km spatial and daily temporal resolutions) dataset of 11 years (2003 to 2013) remotely sensed SST by MODIS sensor onboard Aqua and Terra satellites has been investigated and compared with coastal numerical model experiments. The detection and characterization fronts with fluctuating amplitudes is achieved through the Singularity Analysis (i.e. the process of calculating the degree of regularity or irregularity of a function at each point in a domain).

Publication: [18].

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## 7.7. Pathological speech processing

Participants: K. Daoudi, G. Li, Q. Robin, F. G. Satsou.

- Small amount of training data in learning robust classifiers for differential diagnosis between progressive supranuclear palsy (PSP) and multiple system atrophy (MSA). We showed that factorial discriminant analysis and logistic regression can lead to such robust classifiers. Moreover, we showed that these models provide good insights on the multivariate variability and (un)correlation of acoustic features, which can facilitate clinical interpretation.
- We investigated the problem of extracting ground thruth of glottal closure instants (GCI) from electroglottographic (EGG) signals of healthy and pathological speakers. We carried out a large experimental study which showed that existing methods are not robust to recording settings and material. We then proposed a method to overcome this problem. On the other hand, this problem highlighted the non robustness of state of the art methods in automatic detection of GCI from speech.
- We made an experimental evaluation of state of the art methods in automatic extraction of the excitation source from voiced speech. To carry out this evaluation, we used a very recent source-filter model of sustained phonations. The results showed that these methods are reliable only in very particular cases and fail in most.
- Matching pursuit (MP), particularly using the Gammatones dictionary, has become a popular tool
  in sparse representations of speech/audio signals. The classical MP algorithm does not however
  take into account psychoacoustical aspects of the auditory system. Recently two algorithms, called
  PAMP and PMP have been introduced in order to select only perceptually relevant atoms during
  MP decomposition. We compared the performance these two algorithms on few speech sentences.
  The results showed that PMP, which also has the strong advantage of including an implicit stop
  criterion, always outperforms PAMP as well as classical MP. We then raised the question of whether
  the Gammatones dictionary is the best choice when using PMP. We thus compared it to the popular
  Gabor and damped-Sinusoids dictionaries. The results showed that Gammatones always outperform
  damped-Sinusoids, and that Gabor yield better reconstruction quality but with higher atoms rate.

Publications: [22], [23], [21], [19].

## **INOCS Team**

# 7. New Results

### 7.1. 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 [21].

**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 [22].

**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 [24].

**Distribution network configuration problems:** A distribution network is a system aiming to transfer a certain type of resource from feeders to customers. Feeders are producers of a resource and customers have a certain demand in this resource that must be satisfied. Distribution networks can be represented on graphs and be subject to constraints that limit the number of intermediate nodes between some elements of the network (hop constraints) because of physical constraints. We used layered graphs for hop constrained problems to build extended formulations [16]. Preprocessing techniques allowed to reduce the size of the layered graphs used. The model was studied on the hop-constrained minimum margin problem in an electricity network. This problem consists of designing a connected electricity distribution network, and to assign customers to electricity feeders at a maximum number of hops so as to maximize the minimum capacity margin over the feeders to avoid an overload for any feeder.

**Comparison of formulations and solution methods for location problems:** We addressed two classes of location problems the Discrete Ordered Median Problem (DOMP) and the two-level uncapacitated facility location problem with single assignment constraints (TUFLP-S), an extension of the uncapacitated facility location problem. We presented several new formulations for the 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 [28]. We also addressed the TUFLP-S for which we presented six mixed-integer programming models based on reformulation techniques and on the relaxation of the integrality of some of the variables associated with location decisions. We compared the models by carrying out extensive computational experiments on large, hard, artificial instances, as well as on instances derived from an industrial application in freight transportation [27].

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 over a large planning horizon, the driver/trailer allocation management. Clearly, this problem is an optimization problem with complex structure, for which we propose an extended formulation that we address with a heuristic branch-price-and-cut method. Among the difficulties, that we had to face, are: the fractional objective function, the simultaneous generation of constraints and columns, and a complex pricing problem. We evaluate our approach on the benchmark instances proposed by the enterprise Air Liquide co-organiser of challenge. The solution method allowed the team including INOCS members to win the scientific prize of the ROADEF/EURO challenge 2016 [47]. We also addressed a rich Traveling Salesman Problem with Profits encountered in several real-life cases. We proposed a unified solution approach based on variable neighborhood search. Our approach includes two loading neighborhoods based on the solution of mathematical programs are proposed to intensify the search. They interact with the routing neighborhoods as it is commonly done in matheuristics. The performance of the proposed matheuristic is assessed on various instances proposed for the Orienteering Problem and the Orienteering Problem with Time Window including up to 288 customers. The computational results show that the proposed matheuristic is very competitive compared with the state-of-the-art methods. Extensive computational experiments on the new testbed confirm the efficiency of the matheuristic [30].

A heuristic approach to solve an integrated warehouse order picking problem: We study an integrated warehouse order picking problem with manual picking operations. The picking area of the warehouse is composed by a set of storage positions. The working day is divided in periods. For each period, each position contains several pieces of a unique product, and a set of customer orders has to be prepared. An order is a set of products, each associated with a quantity. The order pickers can prepare up to K parcels in a given picking route. The problem consists in jointly deciding: (1) the assignment of references to storage positions in the aisles which need to be filled up; (2) the division of orders into several parcels, respecting weight and size constraints; (3) the batching of parcels into groups of size K, that implicitly define the routing into the picking area. The objective function is to minimize the total walking distance. In order to deal with industrial instances of large size (considering hundreds of clients, thousands of positions and product references) in a short computation time, a heuristic method based on dynamic programming and minimum cost flow paradigms is proposed. Experimental results on an industrial benchmark have reported very good results with respect to the actual industrial solution [64].

**New models for Load Scheduling for Residential Demand Response on Smart Grids.** The residential load scheduling problem is concerned with finding an optimal schedule for the operation of residential loads so as to minimize the total cost of energy while aiming to respect a prescribed limit on the power level of the residence. We propose a mixed integer linear programming formulation of this problem that accounts for the consumption of appliances, generation from a photovoltaic system, and the availability of energy storage. A distinctive feature of our model is the use of operational patterns that capture the individual operational characteristics of each load, giving the model the capability to accommodate a wide range of possible operating

patterns for the flexible loads. The proposed formulation optimizes the choice of operational pattern for each load over a given planning horizon. In this way, it generates a schedule that is optimal for a given planning horizon, unlike many alternatives based on controllers. The formulation can be incorporated into a variety of demand response systems, in particular because it can account for different aspects of the cost of energy, such as the cost of power capacity violations, to reflect the needs or requirements of the grid. Our computational results show that the proposed formulation is able to achieve electricity costs savings and to reduce peaks in the power consumption, by shifting the demand and by efficiently using a battery [52].

Lagrangian heuristics for SVM with feature selection: The focus of pattern classification is to recognize similarities in the data, categorizing them in different subsets. In many fields, such as the financial and the medical ones, classification of data (samples in Machine Learning language) is useful for analysis or diagnosis purposes. Quite often datasets are formed by a small number of samples, which in turn are characterized by a huge number of attributes (features). The handling of the entire feature set would be computationally very expensive and its outcome would lack from insight. For this reason, it is convenient to reduce the set of features which is expected to be easier to interpret and also easy to evaluate. However, it is not always easy to predict which of those are relevant for classification purposes. Hence it is necessary to screen off the relevant features from those which are irrelevant. The process that selects the features entering the subset of the relevant ones is known as Feature Selection (FS). The (FS) problem can be treated explicitly as a Mixed Binary Programming (MBP) one in the framework of the Support Vector Machine approach. We have discussed a Lagrangianrelaxation-based heuristics. In particular we embed into our objective function a weighted combination of the  $L^1$  and  $L^0$  norm of the normal to the separating hyperplane. We come out with a Mixed Binary Linear Programming problem which is suitable for a Lagrangian relaxation approach. Based on a property of the optimal multiplier setting, we apply a consolidated nonsmooth optimization ascent algorithm to solve the resulting Lagrangian dual. In the proposed approach we get, at every ascent step, both a lower bound on the optimal solution as well as a feasible solution at low computational cost [26].

**Decomposition methods for tree-based network design problems:** We studied different problems, where the underlying solution structure needs to have a tree-like topology and some additional constraints need to be fulfilled. For all these problems, we focused on solution approaches, which allow to tackle large-scale instances, as the application of these problems in areas like systems biology often has to deal with instances containing tens of thousands of nodes. In order to solve these problems efficiently, we turned to decomposition methods, like Benders decomposition, Lagrangian relaxation or relax-and-cut. The considered problems include the (prize-collecting) Steiner tree problem [17], [33], tree-star problems [32], the shared arborescence problem [34], the upgrading spanning tree problem [36] and for maximum-weight connected subgraph problems [35].

We also studied models arising in the design of switched Ethernet networks implementing the Multiple Spanning Tree Protocol [24]. In these problems, multiple spanning trees have to be established in a network to route demands partitioned into virtual local access networks. Different mixed-integer formulations for the problem have been proposed and compared, both theoretically and computationally.

**Dynamic programming for the minimum-cost maximal knapsack packing problem:** Given a set of items with profits and weights and a knapsack capacity, we studied the problem of finding a maximal knapsack packing that minimizes the profit of the selected items. We proposed an effective dynamic programming (DP) algorithm which has a pseudo-polynomial time complexity. We demonstrated the equivalence between this problem and the problem of finding a minimal knapsack cover that maximizes the profit of the selected items. In an extensive computational study on a large and diverse set of benchmark instances, we demonstrated that the new DP algorithm outperforms a state-of-the-art commercial mixed-integer programming (MIP) solver applied to the two best performing MIP models from the literature [25].

## 7.2. 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. Moreover the follower is able to produce renewable energy and store it. The pricing problems, we model, belong to the category of stochastic single leader single follower problems. A scenario based approach is based to solve the problem. For each scenario, the bilevel program is solved by rewriting it as a single level optimization program. 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 [53].

**Network pricing problems with unit toll:** In the so-called network pricing problem an authority owns some arcs of the network and tolls them, while users travel between their origin and destination choosing their minimum cost path. We consider a unit toll scheme, and in particular the cases where the authority is imposing either the same toll on all of its arcs, or a toll proportional to a given parameter particular to each arc (for instance a per kilometer toll). We show that if tolls are all equal then the complexity of the problem is polynomial, whereas in case of proportional tolls it is pseudo-polynomial, proposing ad-hoc solution algorithms and relating these problems to the parametric shortest path problem. We then address a robust approach using an interval representation to take into consideration uncertainty on parameters. We show how to modify the algorithms for the deterministic case to solve the robust counterparts, maintaining their complexity class [15].

**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 identify 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 [66].

A branch and price algorithm for solving Stackelberg Security games: Mixed integer optimization formulations are an attractive alternative to solve Stackelberg Game problems thanks to the efficiency of state of the art mixed integer algorithms. In particular, decomposition algorithms, such as branch and price methods, make it possible to tackle instances large enough to represent games inspired in real world domains. We focus on Stackelberg Games that arise from a security application and investigate the use of a new branch and price method to solve its mixed integer optimization formulation. We prove that the algorithm provides upper and lower bounds on the optimal solution at every iteration and investigate the use of stabilization heuristics. Our preliminary computational results compare this solution approach with previous decomposition methods obtained from alternative integer programming formulations of Stackelberg games [29].

A new general-purpose algorithm for mixed-integer bilevel linear programs: We considered bilevel problems with continuous and discrete variables at both levels, with linear objectives and constraints (continuous upper level variables, if any, must not appear in the lower level problem). We proposed a general-purpose branch-and-cut exact solution method based on several new classes of valid inequalities, which also exploits a very effective bilevel-specific preprocessing procedure. An extensive computational study was presented to evaluate the performance of various solution methods on a common testbed of more than 800 instances from the literature and 60 randomly generated instances. Our new algorithm consistently outperformed (often by a large margin) alternative state-of-the-art methods from the literature, including methods exploiting problem-specific information for special instance classes. In particular, it solved to optimality more than 300 previously unsolved instances from the literature. To foster research on this challenging topic, our solver was made publicly available online [18], [19].

A mixed-integer programming based heuristic for generalized interdiction problems: We considered a subfamily of mixed-integer linear bilevel problems that we call Generalized Interdiction Problems. This class of problems includes, among others, the widely-studied interdiction problems, i.e., zero-sum Stackelberg games where two players (called the leader and the follower) share a set of items, and the leader can interdict the usage of certain items by the follower. Problems of this type can be modeled as Mixed-Integer Nonlinear Programming problems, whose exact solution can be very hard. We propose a new heuristic scheme based on a single-level and compact mixed-integer linear programming reformulation of the problem obtained by relaxing the integrality of the follower variables. A distinguished feature of our method is that general-purpose mixed-integer cutting planes for the follower problem are exploited, on the fly, to dynamically improve the reformulation. The resulting heuristic algorithm proved very effective on a large number of test instances, often providing an (almost) optimal solution within very short computing times. [20]

**Unit Commitment under Market Equilibrium Constraints:** Traditional (deterministic) models for the Unit Commitment problem (UC) assume that the net demand for each period is perfectly known in advance, or in more recent and more realistic approaches, that a set of possible demand scenarios is known (leading to stochastic or robust optimization problems). However, in practice, the demand is dictated by the amounts that can be sold by the producer at given prices on the day-ahead market. We modeled and solved the UC problem with a second level of decisions ensuring that the produced quantities are cleared at market equilibrium. In its simplest form, we are faced to a bilevel optimization problem where the first level is a MIP and the second level linear. As a first approach to the problem, we assumed that demand curves and offers of competitors in the market are known to the operator. Following the classical approach for these models, we turned the problem into a single-level program by rewriting and linearizing the first-order optimality conditions of the second level [50].

### 7.3. 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. Moreover, we addressed the operational planning problem which aims to incorporate the tactical master plan solutions into the realtime allocation of client requests to the couriers. We proposed a mathematical model and a solution approach based on a column generation algorithm. The goal of this approach was to provide a tool to evaluate the robustness of the tactical plan, i.e. how well this plan reacts to new order requests arriving in real-time. 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 [38], [65].

**Decomposition method for the stochastic Steiner tree problem:** We introduced a new algorithmic approach for solving the stochastic Steiner tree problem based on three procedures for computing lower bounds (dual ascent, Lagrangian relaxation, Benders decomposition). Our method is derived from a new integer linear

programming formulation, which is shown to be strongest among all known formulations. The resulting method, which relies on an interplay of the dual information retrieved from the respective dual procedures, computes upper and lower bounds and combines them with several rules for fixing variables in order to decrease the size of problem instances. The effectiveness of our method is compared in an extensive computational study with the state-of-the-art exact approach, which employs a Benders decomposition based on two-stage branch-and-cut, and a genetic algorithm introduced during the DIMACS implementation challenge on Steiner trees. Our results indicate that the presented method significantly outperforms existing ones, both on benchmark instances from literature, as well as on large-scale telecommunication networks [31].

## **MISTIS Project-Team**

## 7. New Results

### 7.1. Mixture models

# 7.1.1. Robust and collaborative extensions of Sliced Inverse Regression.

Participants: Stéphane Girard, Florence Forbes.

This research theme was supported by a LabEx PERSYVAL-Lab project-team grant.

Joint work with: A. Chiancone and J. Chanussot (Gipsa-lab and Grenoble-INP).

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 [16], we investigate the properties of 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.

For further improvement of SIR, in his PhD thesis work, Alessandro Chiancone studied the extension of the SIR method to different sub-populations. The idea is to assume that the dimension reduction subspace is not the same for different clusters of the data [17]. One of the difficulties 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 clusters 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.

### 7.1.2. Structured mixture of linear mappings in high dimension

Participant: Florence Forbes.

**Joint work with:** Benjamin Lemasson from Grenoble Institute of Neuroscience, Naisyin Wang and Chun-Chen Tu from University of Michigan, Ann Arbor, USA.

Regression is a widely used statistical tool. A large number of applications consists of learning the association between responses and predictors. From such an association, different tasks, including prediction, can then be conducted. To go beyond simple linear models while maintaining tractability, non-linear mappings can be handled through exploration of local linearity. The non-linear relationship can be captured by a mixture of locally linear regression models as proposed in the so-called Gaussian Locally Linear Mapping (GLLiM) model [6] that assumes Gaussian noise models. GLLiM is based on a joint modeling of both the responses and covariates, observed or latent. This joint modeling allows for the use of an inverse regression strategy to handle the high dimensionality of the data. Mixtures are used to approximate non-linear associations. GLLiM groups data with similar linear association together. Within the same cluster, the association can be considered as locally linear, which can then be resolved under the classical linear regression setting (see Figure 2 (a)). However, when the covariate dimension is much higher than the response dimension, GLLiM may result in erroneous clusters at the low dimension (eg Figure 2 (b)), leading to potentially inaccurate

predictions. Specifically, when the clustering is conducted at a high joint dimension, the distance at low dimension between two members of the same cluster (component) could remain large. As a result, a mixture component might contain several sub-clusters and/or outliers, violating the model Gaussian assumption. This results in a model misspecification effect that can seriously impact prediction performance. A natural way to lessen this effect is to increase the number of components in the mixture making each linear mapping even more local. But this also increases the number of parameters to estimate and therefore requires to be done in a parsimonious manner to avoid over-parameterization. In this work, we propose a parsimonious approach which we refer to as Structured Mixture of Gaussian Locally Linear Mapping (SMoGLLiM) to solve the aforementioned problems. It follows a two-layer hierarchical clustering structure where local components are grouped into global components sharing the same high-dimensional noise covariance structure, which effectively reduces the number of parameters of the model. SMoGLLiM also includes a pruning algorithm for eliminating outliers as well as determining an appropriate number of clusters. Moreover, the number of clusters and training outliers determined by SMoGLLiM can be further used by GLLiM for improving prediction performance. As an extension, a subsetting and parallelization techniques are discussed for the efficiency concern. A preliminary version of this work was presented at the American Statistical Association Joint Statistical Meeting in Baltimore USA in July 2017, [35].



Figure 2. illustration of the GLLiM model: (Top) Non linear relationship approximated as a mixture of locally linear mappings; (Bottom) problematic clustering with a non Gaussian component (orange region) due to unbalanced weights between the high dimensional responses and low dimensional covariates.

### 7.1.3. Dictionary-free MR fingerprinting parameter estimation via inverse regression

Participants: Florence Forbes, Fabien Boux, Julyan Arbel.

Joint work with: Emmanuel Barbier from Grenoble Institute of Neuroscience.

Magnetic resonance imaging (MRI) can map a wide range of tissue properties but is often limited to observe a single parameter at a time. In order to overcome this problem, Ma et al. introduced magnetic resonance fingerprinting (MRF), a procedure based on a dictionary of simulated couples of signals and parameters. Acquired signals called fingerprints are then matched to the closest signal in the dictionary in order to estimate parameters. This requires an exhaustive search in the dictionary, which even for moderately sized problems, becomes costly and possibly intractable . We propose an alternative approach to estimate more parameters at a time. Instead of an exhaustive search for every signal, we use the dictionary to learn the functional relationship between signals and parameters. This allows the direct estimation of parameters without the need of searching through the dictionary. We investigated the use of GLLiM that bypasses the problems associated with high-to-low regression. The experimental validation of our method is performed in the context of vascular fingerprinting could benefit from a regression approach to limit dictionary size and fasten computation time. Preliminary tests and results have been submitted to ISMRM 2018, International Society for Magnetic Resonance in Medicine.

### 7.1.4. Semiparametric copula-based clustering

Participants: Florence Forbes, Gildas Mazo, Yaroslav Averyanov.

Modeling of distributions mixtures has rested on Gaussian distributions and/or a conditional independence hypothesis for a long time. Only recently have researchers begun to construct and study broader generic models without appealing to such hypotheses. Some of these extensions use copulas as a tool to build flexible models, as they permit to model the dependence and the marginal distributions separately. Recently [70], a semiparametric copula-based mixture model has been proposed to cluster continuous data. This semiparametric feature allows for more flexibility and reduces the modelling effort for the practitioner. Nonetheless, these advantages come at the cost of assuming that the clusters do not differ in scale. The aim of the internship of Y. Averyanov was to get rid of this assumption by building a nonparametric estimator which have to satisfy certain moment constraints. The performance of the estimator was tested on simulations and then embedded into an EM-like algorithm framework.

# 7.1.5. Fully automatic lesion localization and characterization: application to brain tumors using multiparametric quantitative MRI data

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Emmanuel Barbier, Nora Collomb and Benjamin Lemasson from Grenoble Institute of Neuroscience.

When analyzing brain tumors, two tasks are intrinsically linked, spatial localization and physiological characterization of the lesioned tissues. Automated data-driven solutions exist, based on image segmentation techniques or physiological parameters analysis, but for each task separately, the other being performed manually or with user tuning operations. In this work, the availability of quantitative magnetic resonance (MR) parameters is combined with advanced multivariate statistical tools to design a fully automated method that jointly performs both localization and characterization. Non trivial interactions between relevant physiological parameters are captured thanks to recent generalized Student distributions that provide a larger variety of distributional shapes compared to the more standard Gaussian distributions. Probabilistic mixtures of the former distributions are then considered to account for the different tissue types and potential heterogeneity of lesions. Discriminative multivariate features are subsequently pooled together to build a statistical fingerprint model of the different lesion types that captures lesion characteristics while accounting for inter-subject variability. The potential of this generic procedure is demonstrated on a data set of 53 rats, with 36 rats bearing 4 different brain tumors, for which 5 quantitative MR parameters were acquired. This study has been submitted for publication [15].

Analyzing brain tumor tissue composition can then 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 have been 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. This work has been presented at ISMRM 2017, International Society for Magnetic Resonance in Medicine [42].

#### 7.1.6. Signature extraction in MR scans for de novo Parkinsonian patients

Participants: Florence Forbes, Veronica Munoz Ramirez, Julyan Arbel.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience.

This work is part of the cross-disciplinary project NeuroCoG. Parkinson's disease (PD) is characterized by the degeneration of dopaminergic neurons located in the substantia nigra pars compacta (SNc). This leads to well-known motor symptoms associated to Parkinson's disease, rigidity, akinesia and tremor. However, non-motor symptoms also appear. It is of primordial interest to understand these symptoms in order to optimize treatments and diagnose at an early stage the pathology's occurrence. The goal of the PhD work of Veronica Munoz Ramirez is the extraction of specific signatures from MR data of de novo PD patients. We investigated the possibility to use multivariate non-supervised clustering techniques as developed in the PhD thesis of Alexis Arnaud to cluster voxels taking into account interactions between various parameters.

## 7.1.7. Object-based classification from high resolution satellite image time series with Gaussian mean map kernels

Participant: Stéphane Girard.

Joint work with: C. Bouveyron (Univ. Paris 5), M. Fauvel and M. Lopes (ENSAT Toulouse)

In the PhD work of Charles Bouveyron [65], 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 [22], [23], 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. To measure the similarity between two grasslands, a new kernel is proposed as a second contribution: the a-Gaussian mean kernel. It allows to weight the influence of the covariance matrix when comparing two Gaussian distributions. This kernel is introduced in Support Vector Machine for the supervised classification of grasslands from southwest France. A dense intra-annual multispectral time series of Formosat-2 satellite is used for the classification

of grasslands management practices, while an inter-annual NDVI time series of Formosat-2 is used for permanent and temporary grasslands discrimination. Results are compared to other existing pixel- and objectbased approaches in terms of classification accuracy and processing time. The proposed method shows to be a good compromise between processing speed and classification accuracy. It can adapt to the classification constraints and it encompasses several similarity measures known in the literature. It is appropriate for the classification of small and heterogeneous objects such as grasslands.

## 7.2. Semi and non-parametric methods

### 7.2.1. Robust estimation for extremes

Participants: Clément Albert, Stéphane 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 and we investigate their extrapolation ability [36], [37]. To reduce this sensitivity, robust methods are needed and 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: Stéphane 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 [67] with extreme-value methods in order to obtain efficient estimators of the conditional tail index and conditional extreme quantiles [61].

### 7.2.3. Estimation of extreme risk measures

Participant: Stéphane Girard.

**Joint work with:** A. Daouia (Univ. Toulouse), L. Gardes (Univ. Strasbourg), J. Elmethni (Univ. Paris 5) and G. Stupfler (Univ. Nottingham, UK).

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  $\alpha$ -quantile of the loss distribution. The Value-at-Risk however suffers from several weaknesses. First, it provides us only with a pointwise information: VaR( $\alpha$ ) 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  $\alpha$ -quantile of the loss distribution. In [61], 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 [18]. 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 [19] 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. Level sets estimation

Participant: Stéphane Girard.

Joint work with: G. Stupfler (Univ. Nottingham, UK).

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 that the so-called geometric quantiles have very counter-intuitive properties in such situations [21] and thus should not be used to detect outliers.

### 7.2.5. Approximate Bayesian inference

Participant: Julyan Arbel.

Joint work with: Igor Prünster, Stefano Favaro.

Approximate Bayesian inference was tackled from two perspectives.

First, from a computational viewpoint, we have proposed an algorithm which allows for controlling the approximation error in Bayesian nonparametric posterior sampling. In [14], we show that completely random measures (CRM) represent the key building block of a wide variety of popular stochastic models and play a pivotal role in modern Bayesian Nonparametrics. The popular Ferguson & Klass representation of CRMs as a random series with decreasing jumps can immediately be turned into an algorithm for sampling realizations of CRMs or more elaborate models involving transformedCRMs. However, concrete implementation requires to truncate the random series at some threshold resulting in an approximation error. The goal of this work is to quantify the quality of the approximation by a moment-matching criterion, which consists in evaluating a measure of discrepancy between actual moments and moments based on the simulation output. Seen as a function of the truncation level, the methodology can be used to determine the truncation level needed to reach a certain level of precision. The resulting moment-matching Ferguson & Klass algorithm is then implemented and illustrated on several popular Bayesian nonparametric models.

In [57], we focus on the truncation error of a superposed gamma process in a decreasing order representation. As in [14], we utilize the constructive representation due to Ferguson and Klass which 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 momentmatching 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.

Second, we have proposed an approximation of Gibbs-type random probability measures at the level of the predictive probabilities. Gibbs-type random probability measures are arguably the most "natural" generalization of the Dirichlet process. Among them the two parameter Poisson–Dirichlet process certainly stands out for the mathematical tractability and interpretability of its predictive probabilistic models for linguistic applications, e.g., machine learning theory, probabilistic models for linguistic applications, Bayesian nonparametric statistics, excursion theory, measure-valued diffusions in population genetics, combinatorics and statistical physics. Given a sample of size n, in this work we show that the predictive probabilities of any Gibbs-type prior admit a large n approximation, with an error term vanishing as o(1/n), which maintains the same desirable features as the predictive probabilities of the two parameter Poisson–Dirichlet prior.

### 7.2.6. Bayesian nonparametric posterior asymptotic behavior

Participant: Julyan Arbel.

Joint work with: Olivier Marchal, Stefano Favaro, Bernardo Nipoti, Yee Whye Teh.

In [24], we obtain the optimal proxy variance for the sub-Gaussianity of Beta distribution, thus proving upper bounds recently conjectured by Elder (2016). We provide different proof techniques for the symmetrical (around its mean) case and the non-symmetrical case. The technique in the latter case relies on studying the ordinary differential equation satisfied by the Beta moment-generating function known as the confluent hypergeometric function. As a consequence, we derive the optimal proxy variance for the Dirichlet distribution, which is apparently a novel result. We also provide a new proof of the optimal proxy variance for the Bernoulli distribution, and discuss in this context the proxy variance relation to log-Sobolev inequalities and transport inequalities.

The article [13] deals with a Bayesian nonparametric inference for discovery probabilities: credible intervals and large sample asymptotics. Given a sample of size n from a population of individual belonging to different species with unknown proportions, a popular problem of practical interest consists in making inference on the probability  $D_n(l)$  that the (n + 1)-th draw coincides with a species with frequency l in the sample, for any l = 0, 1, ..., n. We explore in this work a Bayesian nonparametric viewpoint for inference of  $D_n(l)$ . Specifically, under the general framework of Gibbs-type priors we show how to derive credible intervals for the Bayesian nonparametric estimator of  $D_n(l)$ , and we investigate the large n asymptotic behavior of such an estimator. We also compare this estimator to the classical Good–Turing estimator.

### 7.2.7. A Bayesian nonparametric approach to ecological risk assessment Participant: Julyan Arbel.

Joint work with Guillaume Kon Kam King, Igor Prünster.

We revisit a classical method for ecological risk assessment, the Species Sensitivity Distribution (SSD) approach, in a Bayesian nonparametric framework. SSD is a mandatory diagnostic required by environmental regulatory bodies from the European Union, the United States, Australia, China etc. Yet, it is subject to much scientific criticism, notably concerning a historically debated parametric assumption for modelling species variability. Tackling the problem using nonparametric mixture models, it is possible to shed this

parametric assumption and build a statistically sounder basis for SSD. We use Normalized Random Measures with Independent Increments (NRMI) as the mixing measure because they offer a greater flexibility than the Dirichlet process. Indeed, NRMI can induce a prior on the number of components in the mixture model that is less informative than the Dirichlet process. This feature is consistent with the fact that SSD practitioners do not usually have a strong prior belief on the number of components. In this work, we illustrate the advantage of the nonparametric SSD over the classical normal SSD and a kernel density estimate SSD on several real datasets[59].

### 7.2.8. Machine learning methods for the inversion of hyperspectral images

Participant: Stéphane Girard.

Joint work with: S. Douté (IPAG, Grenoble), M. Fauvel (INRA, Toulouse) and L. Gardes (Univ. Strasbourg).

We address the physical analysis of planetary hyperspectral images by massive inversion [58]. A direct radiative transfer model that relates a given combination of atmospheric or surface parameters to a spectrum is used to build a training set of synthetic observables. The inversion is based on the statistical estimation of the functional relationship between parameters and spectra. To deal with high dimensionality (image cubes typically present hundreds of bands), a two step method is proposed, namely K-GRSIR. It consists of a dimension reduction step followed by a regression with a non-linear least-squares algorithm. The dimension reduction is performed with the Gaussian Regularized Sliced Inverse Regression algorithm, which finds the most relevant directions in the space of synthetic spectra for the regression. The method is compared to several algorithms: a regularized version of k-nearest neighbors, partial least-squares, linear and non-linear support vector machines. Experimental results on simulated data sets have shown that non-linear support vector machines is the most accurate method followed by K-GRSIR. However, when dealing with real data sets, K-GRSIR gives the most interpretable results and is easier to train.

### 7.2.9. Multi sensor fusion for acoustic surveillance and monitoring

Participants: Florence Forbes, Jean-Michel Bécu.

Joint work with: Pascal Vouagner and Christophe Thirard from ACOEM company.

In the context of the DGA-rapid WIFUZ project, we addressed the issue of determining the localization of shots from multiple measurements coming from multiple sensors. The WIFUZ project is a collaborative work between various partners: DGA, ACOEM and HIKOB companies and Inria. 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. As an illustration, the MISTIS contribution is to develop technical and scientific solutions as part of a collaborative protection approach, ideally used to guide the best coordinated response between the different vehicles of a military convoy. Indeed, in the case of an attack on a convoy, identifying the threatened vehicles and the origin of the threat is necessary to organize the best response from all members on the convoy. Thus it will be possible to react to the first contact (emergency detection) to provide the best answer for threatened vehicles (escape, lure) and for those not threatened (suppression fire, riposte fire). We developed statistical tools that make it possible to analyze this information (characterization of the threat) using fusion of acoustic and image data from a set of sensors located on various vehicles. We used Bayesian inversion and simulation techniques to recover multiple sources mimicking collaborative interaction between several vehicles.

### 7.2.10. Extraction and data analysis toward "industry of the future"

Participants: Florence Forbes, Hongliang Lu, Fatima Fofana, Gildas Mazo, Jaime Eduardo Arias Almeida.

Joint work with: J. F. Cuccaro and J. C Trochet from Vi-Technology company.

Industry as we know it today will soon disappear. In the future, the machines which constitute the manufacturing process will communicate automatically as to optimize its performance as whole. Transmitted information essentially will be of statistical nature. In the context of VISION 4.0 project with Vi-Technology, the role of MISTIS is to identify what statistical methods might be useful for the printed circuits boards assembly industry. The topic of F. Fofana's internship was to extract and analyze data from two inspection machines of a industrial process making electronic cards. After a first extraction step in the SQL database, the goal was to enlighten the statistical links between these machines. Preliminary experiments and results on the Solder Paste Inspection (SPI) step, at the beginning of the line, helped identifying potentially relevant variables and measurements (eg related to stencil offsets) to identify future defects and discriminate between them. More generally, we have access to two databases at both ends (SPI and Component Inspection) of the assembly process. The goal is to improve our understanding of interactions in the assembly process, find out correlations between defects and physical measures, generate proactive alarms so as to detect departures from normality.

## 7.3. Graphical and Markov models

### 7.3.1. Fast Bayesian network structure learning using quasi-determinism screening

Participants: Thibaud Rahier, Stéphane Girard, Florence Forbes.

Joint work with: Sylvain Marié, Schneider Electric.

Learning the structure of Bayesian networks from data is a NP-Hard problem that involves an optimization task on a super-exponential sized space. In this work, we show that in most real life datasets, a number of the arcs contained in the final structure can be prescreened at low computational cost with a limited impact on the global graph score. We formalize the identification of these arcs via the notion of quasi-determinism, and propose an associated algorithm that reduces the structure learning to a subset of the original variables. We show, on diverse benchmark datasets, that this algorithm exhibits a significant decrease in computational time and complexity for only a little decrease in performance score.

### 7.3.2. Robust graph estimation

Participants: Karina Ashurbekova, Florence Forbes.

Joint work with: Sophie Achard, CNRS, Gipsa-lab.

Graphs are an intuitive way of representing and visualizing the relationships between many variables. A graphical model is a probabilistic model whose conditional independence or other measures of relationship between random variables is given by a graph. Learning graphical models using their observed samples is an important task, and involves both structure and parameter estimation. Generally, graph estimation consists of several steps. First of all, we do not know the distribution of the real data. But we can do an assumption about this distribution. Then the measure of relationship between variables we are interested in can be chosen based on this assumption. All these measures of relationship are related with elements of the covariance or precision matrices. After estimating the covariance/precision matrix the

final graph can be constructed based on elements of this matrix. A lot of graph estimation methods rely on the Gaussian graphical model, in which the random vector Y is assumed to be Gaussian. Under this assumption, the most popular method is the graphical lasso (glasso). In practice, data may deviate from the Gaussian model in various ways. Outliers and heavy tails frequently occur. Contamination of a handful of variables in a few experiments can lead to a drastically wrong graph. So one of our objective is to deal with heavy tailed data using a new family of multivariate heavy-tailed distributions [8] and infer a graph robust to outliers without having to remove them.

### 7.3.3. Spatial mixtures of multiple scaled t-distributions

Participants: Florence Forbes, Alexis Arnaud.

Joint work with: Steven Quinito Masnada, Inria Grenoble Rhone-Alpes

The goal is to implement an hidden Markov model version of our recently introduced mixtures of non standard multiple scaled *t*-distributions. The motivation for doing that is the application to multiparametric MRI data for lesion analysis. When dealing with MRI human data, spatial information is of primary importance. For our preliminary study on rat data [15], the results without spatial information were already quite smooth. The main anatomical structures can be identified. We suspect the reason is that the measured parameters already contain a lot of information about the underlying tissues. However, introducing spatial information is always useful and is our ongoing work. In the statistical framework we have developed (mixture models and EM algorithm), it is conceptually straightforward to introduce an additional Markov random field. In addition, when using a Markov random field it is easy to incorporate additional atlas information.

# 7.3.4. Spectral CT reconstruction with an explicit photon-counting detector model: a "one-step" approach

Participants: Florence Forbes, Pierre-Antoine Rodesch.

Joint work with: Veronique Rebuffel and Clarisse Fournier from CEA-LETI 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. Recent developments in energy-discriminating Photon-Counting Detector (PCD) enable new horizons for spectral CT. With PCDs, new reconstruction methods take advantage of the spectral information measured through energy measurement bins. However PCDs have serious spectral distortion issues due to charge-sharing, fluorescence escape, pileup effect Spectral CT with PCDs can be decomposed into two problems: a noisy geometric inversion problem (as in standard CT) and an additional PCD spectral degradation problem. The aim of this study is to introduce a reconstruction method which solves both problems simultaneously: a one-step approach. An explicit linear detector model is used and characterized by a Detector Response Matrix (DRM). The algorithm reconstructs two basis material maps from energy-window transmission data. For comparison, we also perform a standard two-step approach: an advanced polynomial decomposition of measured sinograms combined with a filtered-back projection reconstruction. The results demonstrate the potential uses of this method for medical imaging or for non-destructive control in industry. Preliminary results will be presented at the SPIE medical imaging 2018 conference in Houston, USA [44].

### 7.3.5. Non parametric Bayesian priors for hidden Markov random fields

Participants: Florence Forbes, Julyan Arbel, Hongliang Lu.

Hidden Markov random field (HMRF) models are widely used for image segmentation or more generally for clustering data under spatial constraints. They can be seen as spatial extensions of independent mixture models. As for standard mixtures, one concern is the automatic selection of the proper number of components in the mixture, or equivalently the number of states in the hidden Markov field. A number of criteria exist to select this number automatically based on penalized likelihood (eg. AIC, BIC, ICL etc.) but they usually require to run several models for different number of classes to choose the best one. Other techniques (eg. reversible jump) use a fully Bayesian setting including a prior on the class number but at the cost of prohibitive computational times. In this work, we investigate alternatives based on the more recent field of Bayesian nonparametrics. In particular, Dirichlet process mixture models (DPMM) have emerged as promising candidates for clustering applications where the number of clusters is unknown. Most applications of DPMM involve observations which are supposed to be independent. For more complex tasks such as unsupervised image segmentation with spatial relationships or dependencies between the observations, DPMM are not satisfying.

### 7.3.6. Automated ischemic stroke lesion MRI quantification

Participant: Florence Forbes.

**Joint work with:** Senan Doyle (Pixyl), Assia Jaillard (CHUGA), Olivier Heck (CHUGA), Olivier Detante (CHUGA) and Michel Dojat (GIN)

Manual delineation by an expert is currently the gold standard for lesion quantification, but is resourceintensive, suffers from inter-rater and intra-rater variability, and does not scale well to large population cohorts. We develop an automated lesion quantification method to assess the efficacy of cell therapy in patients after ischemic stroke. A high-quality sub-acute and chronic stroke dataset was supplied by HERMES. T1-w and 3D-Flair MRIs were acquired from 20 ischemic stroke patients with MCA infarct at 2 and 6 months postevent. Manual delineation was performed by an expert using the Flair image. We propose an unsupervised method employing a hidden Markov random field, with innovations to address the challenges posed by stroke MR scans. We introduce a probabilistic vascular territory atlas, adapted to the patient-specific data in a joint segmentation and registration framework, to model the potential progression and delimitation of vascular accidents. After segmentation, a good correlation is observed between manual and automated lesion volume delineation for the two time points. We therefore propose an unsupervised method with the hypothesis that such a class of methods is more robust to the diversity of images obtained with different sequence parameters and scanners; a particularly sensitive point for multi-center studies. Interestingly, this approach will be used in the European **RESSTORE** cohort.

# 7.3.7. PyHRF: A python library for the analysis of fMRI data based on local estimation of hemodynamic response function

Participants: Florence Forbes, Jaime Eduardo Arias Almeida, Aina Frau Pascual.

Joint work with: Michel Dojat and Jan Warnking from Grenoble Institute of Neuroscience.

Functional Magnetic Resonance Imaging (fMRI) is a neuroimaging technique that allows the non-invasive study of brain function. It is based on the hemodynamic changes induced by cerebral activity following sensory or cognitive stimulation. The measured signal depends on the variation of blood oxygenation level (BOLD signal) which is related to brain activity: a decrease in deoxyhemoglobin induces an increase in BOLD signal. In fact, the signal is convoluted by the Hemodynamic Response Function (HRF) whose exact form is unknown and fluctuates with various parameters such as age, brain region or physiological conditions. In this work we focused on PyHRF, a software to analyze fMRI data using a joint detection-estimation (JDE) approach. It jointly detects cortical activation and estimates the HRF. In contrast to existing tools, PyHRF estimates the HRF instead of considering it as constant in the entire brain, improving thus the reliability of the results. We investigated a number of real data case to demonstrate that PyHRF was a suitable tool for clinical applications. This implied the definition of guidelines to set some of the parameters required to run the software. We investigated a calibration method by comparing results with the standard SPM software in the case of a fixed HRF. An overview of the package and its performance was presented at the 16th Python in Science Conference (SciPy 2017) in Austin, TX, United States [38].

### 7.3.8. 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: 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 decide whether a text was related or not to a target topic presented to them beforehand. 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 [55]. 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.

New results were obtained in the standalone analysis of the eye-movements. A comparison between the effects of three types of texts was performed, considering texts either closely related, moderately related or unrelated to the target topic.

Our 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.

# **7.3.9.** Markov models for the analysis of the alternation of flowering in apple tree progenies **Participant:** Jean-Baptiste Durand.

This research theme is supported by a Franco-German ANR grant (AlternApp project).

Joint work with: Evelyne Costes (INRA AGAP, AFEF team)

A first study was published to characterize genetic determinisms of the alternation of flowering in apple tree progenies. Data were collected at two scales: at whole tree scale (with annual time step) and a local scale (annual shoots, which correspond to portions of stems that were grown during the same year). One or several replications of each genotype were available.

Three families of indices were proposed for early detection of alternation during the juvenile phase. The first family was based on a trend model and a quantification of the deviation amplitudes and dependency, with respect to the trend. The second family was based on a 2nd-order Markov chain with fixed and random effect in transition probabilities. The third family was based on entropy indices, in which flowering probabilities were corrected from fixed effects using Generalized Linear Models.

This allowed early quantification of alternation from the yearly numbers of inflorescences at tree scale. Some quantitative trait loci (QTL) were found in relation with these indices [40], [20].

New data sets where collected in other F1 progenies. Ancestral relationships between parents of different progenies were taken into account to enhance the power of QTL detection using Bayesian methods. Other QTLs are expected to be found using these new indices and genetic material. However, the amount of replicate per genotype and of data per replicate is quite reduced compared to those of our previous work. This is why we will investigate the loss of power in QTL detection due to a degraded amount of data, by simulating data deletion in our reference results.

## **MODAL Project-Team**

## 7. New Results

## 7.1. An Oracle Inequality for Quasi-Bayesian Non-Negative Matrix Factorization

Participant: Benjamin Guedj.

The quasi-Bayesian perspective has been extended to the popular setting of non-negative matrix factorization. This is a pivotal problem in machine learning (image segmentation, recommendation systems, audio source separation, ...) and an original estimator of the unobserved matrix has been proposed. An oracle inequality is derived, along with several possible implementations. This work is published in Mathematical Methods of Statistics [12].

It a joint work with Pierre Alquier from ENSAE - Université Paris-Saclay.

### 7.2. Simpler PAC-Bayesian Bounds for Hostile Data

Participant: Benjamin Guedj.

An original and much simpler way of deriving PAC-Bayesian bounds has been introduced through the use of f-divergences (therefore generalizing earlier works on Renyi's divergence and Kullback-Leibler divergence). This work is published in Machine Learning [13].

It a joint work with Pierre Alquier from ENSAE - Université Paris-Saclay.

## 7.3. Highlight 1 High-dimensional Adaptive Ranking with PAC-Bayesian Bounds

Participant: Benjamin Guedj.

The quasi-Bayesian perspective has been extended to the popular setting high-dimensional ranking. This is a pivotal problem in machine learning and is at the core of several applications in industry (recommender systems, active learning, ...). An original estimator of the scoring function is proposed, and we have shown its minimax optimal properties. Our procedure is adaptive to the unknown sparsity level of the data. This work is published in Journal of Statistical Planning and Inference.

It a joint work with Sylvain Robbiano from University College London.

### 7.4. Online Adaptive Clustering

Participant: Benjamin Guedj.

The quasi-Bayesian perspective has been extended to online adaptive clustering. Data streams are clustered dynamically with a quasi-Bayesian-flavored predictor, and we have proven minimax regret bounds. An efficient MCMC-based implementation is proposed.

## 7.5. Study of Transcriptional Regulation

Participant: Guillemette Marot.

The implementation of a mixture model of normal and exponential laws enabled to define a threshold on the number of co-recruiting transcriptional regulators in order to classify cis-regulatory modules. The new findings in Biology have been published in [16].

## 7.6. Functional Binary Linear Models for Stratified Samples

Participant: Sophie Dabo-Niang.

Sophie Dabo-Niang's new result concern a work on functional binary linear models for stratified samples. This work introduces a new functional binary choice model in a case-control or choice-based sample design context, where the response is binary, while the explanatory variable is functional. The model is estimated when the sample is stratified with respect to the values of the response variable. A dimensional reduction of the space of the explanatory random function based on a Karhunen-Loève expansion is used to define a conditional maximum likelihood estimate of the model. Based on this formulation, several asymptotic properties are given. Numerical experiments are used to compare the proposed method with the ordinary maximum likelihood method, which ignores the nature of the sampling. The proposed model yields encouraging results.

## 7.7. 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 has been proposed. 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 published to an international journal [18]. Furthermore, an R package (MixCluster) is available on Rforge.

## 7.8. Data Units Selection in Statistics

Participant: Christophe Biernacki.

Usually, the data unit definition is fixed by the practitioner but it can happen that he/her 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, count, categorical). This work is now in revision for an international journal [36]. It has led also to three invitations as a plenary session speaker to international or national conferences (the US Classification Society Conference [27], the French Classification Society Conference [28], the StatLearn conference [20]).

It is a joint work with Alexandre Lourme from University of Bordeaux.

### 7.9. Trade-off Between Computation Time and Accuracy

Participants: Christophe Biernacki, Maxime Brunin, Alain Célisse.

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. This work has been presented to an international conference [20] and a national conference [29], and a preprint is still being in progress.

Maxime Brunin will defend his PhD thesis related to this topic on January 2018.

### 7.10. Projection Under Pairwise Control

Participant: Christophe Biernacki.

Visualization of high-dimensional and possibly complex (non continuous for instance) data onto a lowdimensional 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  $\mathbb{R}^2$  with a simple reading of the approximation quality, and provides then a novel variant of dimensionality reduction.

This work is still under revision in an international journal [39].

It is a joint work with Hiba Alawieh and Nicolas Wicker, both from University of Lille.

## 7.11. 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 6errors on a database composed of 50 classes). This work has been now extended with success to the multi-sources classification case and also the computational load has been sufficiently reduced to reach the real time target (less than 50ms). This work has been presented to an international conference in Signal Processing [25] and also to a national conference [26]. A preprint is well advanced and should be submitted to an international journal at the end of 2017.

It is a joint work with Raphaël Greff, from the A-Volute company.

### 7.12. Model-Based Co-clustering for Ordinal Data

Participant: Christophe Biernacki.

A model-based co-clustering algorithm for ordinal data is presented. This algorithm relies on the latent block model embedding a probability distribution specific to ordinal data (the so-called BOS or Binary Ordinal Search distribution). Model inference relies on a Stochastic EM algorithm coupled with a Gibbs sampler, and the ICL-BIC criterion is used for selecting the number of co-clusters (or blocks). The main advantage of this ordinal dedicated co-clustering model is its parsimony, the interpretability of the co-cluster parameters (mode, precision) and the possibility to take into account missing data. Numerical experiments on simulated data show the efficiency of the inference strategy, and real data analyses illustrate the interest of the proposed procedure. The resulting work is in revision to an international journal [40].

This is joint work Julien Jacques from University of Lyon 2.

### 7.13. Model-Based Co-clustering for Ordinal Data of different dimensions

Participant: Christophe Biernacki.

This work has been motivated by a psychological survey on women affected by a breast tumor. Patients replied at different moments of their treatment to questionnaires with answers on ordinal scale. The questions relate to aspects of their life called dimensions. To assist the psychologists in analyzing the results, it is useful to emphasize a structure in the dataset. The clustering method achieves that by creating groups of individuals that are depicted by a representative of the group. From a psychological position, it is also useful to observe how questions may be grouped. This is why a clustering should be performed also on the features, which is called a co-clustering problem. However, gathering questions that are not related to the same dimension does not make sense from a psychologist stance. Therefore, the present work corresponds to perform a constrained co-clustering method aiming to prevent questions from different dimensions from getting assembled in a same column-cluster. In addition, evolution of co-clusters along time has been investigated. The method relies on a constrained Latent Block Model embedding a probability distribution for ordinal data. Parameter estimation relies on a Stochastic EM-algorithm associated to a Gibbs sampler, and the ICL-BIC criterion is used for selecting the numbers of co-clusters. The resulting work has been submitted to an international journal [42].

This is joint work with Margot Selosse and Julien Jacques, both from University of Lyon 2. Margot Selosse is a new PhD student co-supervised by Julien Jacques and Christophe Biernacki.

## 7.14. MASSICCC Platform for SaaS Software Availability

Participants: Christophe Biernacki, Vincent Kubicki, Jonas Renault, Josselin Demont, Matthieu Marbac.

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

MASSICCC has led to a second short meeting in February 2017 in Lille (after a first short meeting in April 2016 in Lille) for obtaining a feedback from company and academic users.

The MASSICCC platform is available here in the web: https://massiccc.lille.inria.fr

## 7.15. Model-Based Co-Clustering of Multivariate Functional Data

Participant: Christophe Biernacki.

High dimensional data clustering is an increasingly interesting topic in the statistical analysis of heterogeneous large-scale data. We consider the problem of clustering heterogeneous high-dimensional data where the individuals are described by functional variables which exhibit a dynamical longitudinal structure. We address the issue in the framework of model-based co-clustering and propose the functional latent block model (FLBM). The introduced FLBM model allows to simultaneously cluster a sample of multivariate functions into a finite set of blocks, each block being an association of a cluster over individuals and a cluster over functional variables. Furthermore, the homogeneous set within each block is modeled with a dedicated latent process functional regression model which allows its segmentation according to an underlying dynamical structure. The proposed model allows thus to fully exploit the structure of the data, compared to classical latent block clustering models for continuous non functional data, which ignores the functional structure of the observations. The FLBM can therefore serve for simultaneous co-clustering and segmentation of multivariate non-stationary functions. We propose a variational expectation-maximization (EM) algorithm (VEM-FLBM) to monotonically maximize a variational approximation of the observed-data log-likelihood for the unsupervised inference of the FLBM model. This work has been presented as an invited speaker to the 61th World Staistics Congress [30].

This is a joint work with Faicel Chamroukhi of University of Caen.

### 7.16. Reject Inference Methods in Credit Scoring: A Rational Review

Participants: Christophe Biernacki, Adrien Ehrhardt, Vincent Vandewalle.

The granting process of all credit institutions rejects applicants having a low credit score. Developing a scorecard, *i.e.* a correspondence table between a client's characteristics and his score, requires a learning dataset in which the target variable good/bad borrower is known. Rejected applicants are *de facto* excluded from the process. This biased learning population might have deep consequences on the scorecard relevance. Some works, mostly empirical ones, try to exploit rejected applicants in the scorecard building process. This work proposes a rational criterion to evaluate the quality of a scoring model for the existing Reject Inference methods and dig out their implicit mathematical hypotheses. It is shown that, up to now, no such Reject Inference method can guarantee a better credit scorecard. These conclusions are illustrated on simulated and real data from the french branch of Crédit Agricole Consumer Finance (CACF). An early version of this work has been presented as a talk in the national conference [31] and a preprint is being to be finalized.

This is a joint work with Philippe Heinrich of University of Lille and Sébastien Beben of Crédit Agricole Consumer Finance.

## 7.17. Survival Analysis with Complex Covariates: A Model-based Clustering Preprocessing Step

Participants: Christophe Biernacki, Vincent Vandewalle.

Many covariates are now available through sensors in the industrial context, and are expected to be related to the survival analysis target. Such covariates are often complex, what has to be understood as a possible mix between continuous, categorical, even functional over time, variables with the possibility to contain missing or uncertain values. A natural question in survival analysis is to design in both flexible and easy way an hazard function related to these potentially complex covariates, while preserving the opportunity to benefit from classical hazard functions.

In the context of a bilateral contract with Alstom company on the survival analysis topic, we have been invited to give a tutorial in the IEEE PHM International Conference on Prognostics and Health Management in US [22]. In this tutorial, we have described how to decompose the unknown targeted hazard function into two complementary parts. The first one can be any classical user hazard function conditional on a latent categorical variable. The second one is the distribution of this latent variable conditionally to the complex covariates. The way to combine both parts is to sum their product over the latent variable (marginal distribution), leading to the final targeted hazard function. The key to perform this approach is to focus on the latent variable definition which can be obtained with a model-based clustering approach dedicated to complex covariates. Beyond a selected review of recent methodologies dedicated to clustering, we have described in depth some related software to perform previous clustering methods. Some case studies have been also provided in an industrial context. At the end of the talk the practitioner is thus able to perform such clustering method to use it finally with its own hazard function.

## 7.18. Dealing with Missing Data Through Mixture Models

Participants: Christophe Biernacki, Vincent Vandewalle.

Many data sets have missing values, however the majority of statistical methods need a complete dataset to work. Thus, practitioners often use imputation or multiple imputations to complete the data as a pre-processing step. Mixture models can be used to naturally deal with missing data in an integrated way depending on the purpose. Especially, they can be used to classify the data or derive estimates for the distances. This work as been presented in an international conference [21].

## 7.19. Review on Mixture Modeling and High-dimensional Clustering

Participant: Christophe Biernacki.

Following the Journées d'Études en Statistique on 2014 in Frejus, on the topic "model choice and model aggregation" where two lectures have been given respectively on mixture model and on high dimensional clustering, a book has been published in 2017 including two chapters related to these talks (respectively [33] and [34]).

The second chapter is a joint work with Cathy Maugis-Rabusseau of INSA Toulouse.

## 7.20. Dealing with Missing Not at Random Values in Model-based Clustering

### Participant: Christophe Biernacki.

Missing values are current in modern data sets. In many situations, making the simplifying hypothesis that they are missing at random is not realistic. However, it is very challenging to propose sensible models which address the underlying missing process. We make such proposals specific to the clustering context, namely making the assumption that missing values are missing at random conditionally to clusters, thus leading to a quite natural not missing at random marginal model. A working paper is in progress.

It is a joint work with Julie Josse of Ecole Polytechnique and Gilles Celeux of Inria Saclay - Île de France.

## 7.21. Dealing with Several Cluster Variables

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, is 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. The behavior of the model is illustrated on simulated and real data. This work as been presented in an international conference [24].

## **RANDOPT Team**

## 6. New Results

### 6.1. Theory

Participants: Anne Auger, Nikolaus Hansen.

The paper "Information-Geometric Optimization Algorithms: A Unifying Picture via Invariance Principles" has finally been published in the JMLR journal [3]. In this paper in collaboration with Yann Ollivier in particular, we lay the ground of stochastic optimization by means of information geometry. We provide a unified framework for stochastic optimization on arbitrary search spaces that allow to recover well-known algorithms on continuous or discrete search spaces and put them under the same umbrella of Information Geometric Optimization.

When analyzing the stability of Markov chains stemming from comparison-based stochastic algorithms, we are facing difficulties due to the fact that the Markov chains have the following form  $\Phi_{t+1} = F(\Phi_t, U_{t+1})$  where  $\{U_t : t \ge 0\}$  are i.i.d. random vectors and F is a discontinuous function. The discontinuity comes from the comparison-based property of the algorithms. If F were  $C^{\infty}$  or  $C^1$  we could prove easily stability properties like irreducibility and show that compact are small sets by investigating the underlying control model and showing that it has globally attracting states where controllability conditions hold using results developed by Sean Meyn and co-authors.

In the paper [2], we found that we can actually generalize to a great extent the results by Meyn to the case where  $\Phi_{t+1} = F(\Phi_t, \alpha(\Phi_t, U_{t+1}))$  where F is  $C^1$  and  $\alpha$  is discontinuous but such that  $\alpha(x, U)$  admits a lower-semi continuity density. We have proposed verifiable conditions for the irreducibility and aperiodicity and shown that compact sets are small sets.

The development of evolution strategies has been greatly driven by so-called progress rate or quality gain analysis where simplification assumptions are made to obtain quantitative estimate of progress in one step and deduce from it how to set different parameters like recombination weights, learning rates ...

This theory while very useful often relied on approximations that were not always well appraised, justified or clearly stated. We have been in the past rigorously deriving different progress rate results and related them to bounds on convergence rates. We have investigated rigorously the quality gain (that is progress measured in terms of objective function) on general convex quadratic functions using weighted recombination. This allowed to derive the dependency of the convergence rate of evolution strategies with respect to the eigenspectrum of the Hessian matrix of convex-quadratic function as well as give hints on how to set learning rate [4] and [9].

## 6.2. Novel Constraint Handling

Participants: Asma Atamna, Anne Auger, Nikolaus Hansen.

In the context of constrained optimization, we have investigated to use augmented Lagrangian approaches to handle constraints. The originality of the approach is that the parameters of the augmented Lagrangian are adapted online. We have shown sufficient conditions for linear convergence of the ensuing methods with linear constraints [5]. Those sufficient conditions rely on finding a Markov chain candidate to be stable. This Markov chain derives from invariance properties of the algorithm. At the same time we have proposed an algorithm variant for the  $(\mu/\mu, \lambda)$ -CMA-ES and an arbitrary number of constraints.

In [10], we have investigated the linear convergence question on the point of view of invariance. We have analyzed the invariances of adaptive algorithms handling constraints with augmented Lagrangian: we have shown that invariance to monotonic transformation of the objective functions is lost but that a subclass of invariance can and should be preserved, namely affine transformation of the objective function and scaling of the constraint by a positive constant.

## 6.3. Benchmarking

Participants: Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Umut Batu, Dejan Tusar.

In his thesis, Ouassim AitElHara has been investigating the benchmarking of algorithms in large dimensions [1]. In this context, the first steps for a testbed of the COCO platform in large dimension have been done. Particularly, the methodology for building a large-scale testbed has been defined: it consists in replacing the usual orthogonal transformation by block-diagonal orthogonal matrices multiplied to the left and to the right by permutation matrices. While still under testing, we expect to be able to release the large-scale testbed in the coming year.

The population size is one of the few parameters, a user is supposed to touch in the state-of-the-art optimizer CMA-ES. In [7], a new approach to also adapt the population size in CMA-ES is proposed and benchmarked on the bbob test suite of our COCO platform. The method is based on tracking the non-decrease of the median of the objective function values in each slot of S successive iterations to decide whether to increase or decrease or keep the population size in the next slot of S iterations. The experimental results show the efficiency of our approach on some multi-modal functions with adequate global structure.

Benchmarking budget-dependent algorithms (for which parameters might depend on the given budget of function evaluations) is typically done for a fixed (set of) budget(s). This, however, has the disadvantage that the reported function values at this budget are difficult to interpret. Furthermore, assessing performance in this way does not give any hints how an algorithm would behave for other budgets. Instead, we proposed in [8] a new way to do "Anytime Benchmarking of Budget-Dependent Algorithms" and implemented this functionality in our COCO platform. The idea is to run several experiments for varying budgets and report target-based runtimes in the form of empirical cumulative distribution functions (aka data profiles) as in the case of anytime algorithms.

### 6.4. Performance Assessment in Multiobjective Optimization

In the context of performance assessment in multiojective optimization, two contributions have been made in 2017. First, we proposed a new visualization method to quantitatively assess the performance of multiobjective optimizers (for 2-objective problems) in the form of average runtime attainment functions [6]. The main idea is to display, for each point in objective space, when (in terms of the average runtime) it has been attained or in other words when it has been dominated by the algorithm. Second, we continued our effort towards automated benchmarking via our COCO platform and described a generic test suite generator that can produce test suites like the previous bbob-biobj test suite for an arbitrary number of objectives<sup>0</sup>.

## 6.5. Comparing Continous Optimizers Platform

Participants: Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Umut Batu, Dejan Tusar.

Thanks to the ADT support for Dejan Tušar (since November, previously supported by ESA) and Umut Batu (since July), as well as due to an increased effort from the core development team, we could progress on several aspects regarding our Comparing Continuous Optimizers platform (COCO, https://github.com/numbbo/coco) in 2017.

Most notably, we provide the new functionality of data archives which allows to access the available data of 200+ algorithms much easier. We also made significant progress towards a first constrained test suite—in particular did we add logging support for constrained problems. The postprocessing module is finally python 3 compatible and zip files are supported as input files. The reference worst f-values-of-interest are exposed to the (multiobjective) solver, algorithms can now be displayed in the background, and simplified example experiment scripts (in python) are available (for both anytime, and budget-dependend algorithms, see also [8]). We also improved our continuous integration support, now using also CircleCI and AppVeyor in addition to Inria's Jenkins system. Version 2.0, released in January 2017, saw new functionality of reference algorithms for the multiobjective test suite, a new format of reference algorithms that allow to use any existing data set

<sup>&</sup>lt;sup>0</sup>Paper to be submitted to the Evolutionary Computation journal and to arXiv/HAL in January 2018.

as reference, improved HTML output and navigation, the COCO version number being part of the plots now, and new regression tests for all provided test suites.

COCO facts for 2017

- 218 issues closed
- major release 2.0 in January plus three additional releases, version 2.2 planned for January 2018
- 10 new contributors outside the main development team
- 14 new algorithm data sets made public (total: 233)

Currently, we are working on an entire rewrite of the postprocessing (ADT COCOpost project of Umut Batu), an improved cocoex module for proposing test suites, functions, data loggers etc. in python (ADT COCOpysuites of Dejan Tušar), a first constrained test suite (in particular Asma Atamna via the PGMO project NumBER), and a large-scale test suite (part of Konstantinos Varelas' PhD thesis, based on the PhD work of Ouassim AitElHara).

Finally, we continued to use COCO also for teaching, in particular for the group project ("controle continue") of our Introduction to Optimization (about 40 Master students) and the Derivative-Free Optimization lectures at Université Paris-Sud (about 30 Master students).

## **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 [15] 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 [17] 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 neighbourhood 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 [13] 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 [16]. 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.

We have developed an algorithm for the exact solution of the Temporal Knapsack Problem [29], [24]. We proposed a dynamic programming formulation for the problem, whose size is exponential in the size of the input data. To cope with the curse of dimensionality, we based our algorithm on the Successive Sublimation Dynamic Programming method. We generalized it to allow more precise aggregation of the state space of the dynamic program. Several application-specific feasibility tests and dominance relations, based on aggregated information, are used to derive an efficient implementation of the method. The algorithms compares favorably with the literature, solving several open instances.

## 7.3. Revisiting Benders Decomposition & Enhancing the Algorithm

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 [98] 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. We have contributed to enhance convergence of Benders cutting plane algorithm by a mixture of smoothing techniques and proximal approaches. Our numerical benchmarking is still on going [18].

## 7.4. 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 [14], [25] 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.

In [36] we deal with the Minimum Latency Problem (MLP), another variant of the well-known Traveling Salesman Problem in which the objective is to minimize the sum of waiting times of customers. This problem arises in many applications where customer satisfaction is more important than the total time spent by the server. This paper presents a novel branch-and-price algorithm for MLP that strongly relies on new features for the ng-path relaxation, namely: (1) a new labeling algorithm with an enhanced dominance rule named multiple partial label dominance; (2) a generalized definition of ng-sets in terms of arcs, instead of nodes; and (3) a strategy for decreasing ng-set sizes when those sets are being dynamically chosen. Also, other elements of efficient exact algorithms for vehicle routing problems are incorporated into our method, such as reduced cost fixing, dual stabilization, route enumeration and strong branching. Computational experiments over TSPLIB instances are reported, showing that several instances not solved by the current state-of-the-art method can now be solved.

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In [37], [31] we consider the Resource Constrained Shortest Path problem arising as a subproblem in stateof-the-art Branch-Cut-and-Price algorithms for vehicle routing problems. We propose a variant of the bidirectional label correcting algorithm in which the labels are stored and extended according to so-called bucket graph. Such organization of labels helps to decrease significantly the number of dominance checks and the running time of the algorithm. We also show how the forward/backward route symmetry can be exploited and how to filter the bucket graph using reduced costs. The proposed algorithm can be especially beneficial for vehicle routing instances with large vehicle capacity and/or with time constraints. Computational experiments were performed on instances from the distance constrained vehicle routing problem, including multi-depot and site-depended variants, on the vehicle routing problem with time windows, and on the "nightmare" instances of the heterogeneous fleet vehicle routing problem. Very significant improvements over the best algorithms in the literature were achieved and many instances could be solved for the first time.

We also considered a family of Vehicle Routing Problem (VRP) variants that generalize the classical Capacitated VRP by taking into account the possibility that vehicles differ by capacity, costs, depot allocation, or even by the subset of customers that they can visit. In [33], [30], [23] we propose a branch-cut-and-price algorithm that adapts advanced features found in the best performing exact algorithms for homogeneous fleet VRPs. The original contributions include: (i) the use of Extended Capacity Cuts, defined over a pseudo-polynomially large extended formulation, together with Rank-1 Cuts, defined over the Set Partitioning Formulation; (ii) the concept of vehicle-type dependent memory for Rank-1 Cuts; and (iii) a new family of lifted Extended Capacity Cuts that takes advantage of the vehicle-type dependent route enumeration. The algorithm was extensively tested in instances of the literature and was shown to be significantly better than previous exact algorithms, finding optimal solutions for many instances with up to 200 customers and also for some larger instances. Several new best solutions were found too.

### 7.5. Machine Scheduling Problems

In [21] we consider the unrelated parallel machine scheduling problem with setup times to minimize a general objective function. In this work we present a novel exact algorithm that is capable of solving this problem  $R|r_j, s_{ij}^k| \sum f_j(C_j)$  and the large class of problems that can be derived as particular cases from it. The proposed algorithm consists of a branch-cut-and-price approach that combines several features such as non-robust cuts, strong branching, reduced cost fixing and dual stabilization. To our knowledge, this is the first exact algorithm for unrelated machines with earliness and/or tardiness criteria that can solve consistently instances with more than 20 jobs. We report improved bounds for instances of problems  $R|r_j, s_{ij}^k| \sum w'_j E_j + w_j T_j$  and  $R||\sum w'_j E_j + w_j T_j$  with up to 80 and 120 jobs, respectively.

## 7.6. Scheduling Strategies for Runtime Systems

We consider the design of low cost but guaranteed approximation algorithms in the context of the runtime StarPU in [20]. In High Performance Computing, heterogeneity is now the norm with specialized accelerators like GPUs providing efficient computational power. The added complexity has led to the development of task-based runtime systems, which allow complex computations to be expressed as task graphs, and rely on scheduling algorithms to perform load balancing between all resources of the platforms. Developing good scheduling algorithms , even on a single node, and analyzing them can thus have a very high impact on the performance of current HPC systems. The special case of two types of resources (namely CPUs and GPUs) is of practical interest. HeteroPrio is such an algorithm which has been proposed in the context of fast multipole computations, and then extended to general task graphs with very interesting results. In this paper, we provide a theoretical insight on the performance of HeteroPrio, by proving approximation bounds compared to the optimal schedule in the case where all tasks are independent and for different platform sizes. Interestingly, this shows that spoliation allows to prove approximation ratios for a list scheduling algorithm on two unrelated resources, which is not possible otherwise. We also establish that almost all our bounds are tight. Additionally, we provide an experimental evaluation of HeteroPrio on real task graphs from dense linear algebra computation, which highlights the reasons explaining its good practical performance.
## 7.7. Matrix Partitioning for Parallel Computing on Heterogeneous Platforms

We consider the combinatorial optimization problem that arises in the context of matrix multiplication in [40]. The problem of partitioning a matrix into a set of sub-matrices has received increased attention recently and is crucial when considering dense linear algebra and kernels with similar communication patterns on heterogeneous platforms. The problem of load balancing and minimizing communication is traditionally reducible to an optimization problem that involves partitioning a square into rectangles. This problem has been proven to be NP-Complete for an arbitrary number of partitions. In this paper, we present recent approaches that relax the restriction that all partitions be rectangles. The first approach uses an original mathematical technique to find the exact optimal partitioning. Due to the complexity of the technique, it has been developed for a small number of partitions only. However, even at a small scale, the optimal partitions found by this approach are often non-rectangular and sometimes non-intuitive. The second approach is the study of approximate partitioning methods by recursive partitioning algorithms. In particular we use the work on optimal partitioning to improve pre-existing algorithms. In this paper we discuss the different perspectives it opens and present two algorithms, SNRPP which is a sqrt(3/2) approximation, and NRPP which is a 2/sqrt(3) approximation. While sub-optimal, this approach works for an arbitrary number of partitions. We use the first exact approach to analyse how close to the known optimal solutions the NRRP algorithm is for small numbers of partitions. In order to validate above approach, we consider in [41] how to allocate data when performing matrix multiplication on a heterogeneous node, with multicores and GPUs. Classical (cyclic) allocations designed for homogeneous settings are not appropriate, but the advent of task-based runtime systems makes it possible to use more general allocations. Previous theoretical work has proposed square and cube partitioning algorithms aimed at minimizing data movement for matrix multiplication. We propose techniques to adapt these continuous square partitionings to allocating discrete tiles of a matrix, and strategies to adapt the static allocation at run-time. We use these techniques in an implementation of Matrix Multiplication based on the StarPU runtime system, and we show through extensive experiments that this implementation allows to consistently obtain a lower communication volume while improving slightly the execution time, compared to standard state-of-the-art dynamic strategies.

## 7.8. Convergence between HPC and Data Science

We consider the use of replication when scheduling independent identical tasks in [34]. MapReduce is a well-know framework for distributing data-processing computations onto 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 split into data chunks that are replicated (a constant number of times, usually 3) and distributed randomly onto computing nodes. During the Map phase, local tasks (i.e., tasks whose data chunks are stored locally) are assigned in priority when processors request tasks. In this paper, we provide the first complete theoretical analysis of data locality in the Map phase of MapReduce, and more generally, for bag-of-tasks applications that behave like MapReduce. We prove that if tasks are homogeneous (in terms of processing time), as soon as the replication factor is larger than 2, FindAssignment, a matching based algorithm, achieves a quasi-perfect makespan (i.e., optimal up to an additive constant of one step) using a sophisticated matching algorithm. Above result is proved with high probability when the number of tasks becomes arbitrarily large, and we therefore complement theoretical results with simulations that corroborate them even for small number of tasks. We also show that the matching-based approach leads to an improvement of data locality during the Map phase and therefore decreases the amount of communications needed to achieve perfect makespan, compared to the classical MapReduce greedy approach. In the context of the convergence between HPC and Data Science, we investigate the use of Burst Buffers for HPC applications in [38]. Burst-Buffers are high throughput, small size intermediate storage systems typically based on SSDs or NVRAM that are designed to be used as a potential buffer between the computing nodes of a supercomputer and its main storage system consisting of hard drives. Their purpose is to absorb the bursts of I/O that many HPC applications experience (for example for saving checkpoints or data from intermediate results). In this paper, we propose a probabilistic model for evaluating the performance of Burst-Buffers. From a model of application and a data management strategy, we build a Markov chain based model of the system, that allows to quickly answer issues about dimensioning of the system: for a given set of applications, and for a given Burst-Buffer size and bandwidth, how often does the buffer overflow? We also provide extensive simulation results to validate our modeling approach.

## 7.9. 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 [22], we design a Two-Echelon Distribution Network that helps synchronise 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.

## 7.10. Two-dimensional Guillotine Cutting Problems

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 [13], 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.

Also we consider a variant of two-dimensional guillotine cutting-stock problem that arises when different bills of order (or batches) are considered consecutively. The raw material leftover of the last cutting pattern is not counted as waste as it can be reused for cutting the next batch. The objective is thus to maximize the length of the leftover. In [35], [32] we propose a diving heuristic based on a Dantzig-Wolfe reformulation solved by column generation in which the pricing problem is solved using dynamic programming (DP). This DP generates so-called non-proper columns, *i.e.* cutting patterns that cannot participate in a feasible integer solution of the problem. We show how to adapt the standard diving heuristic to this "non-proper" case while keeping its effectiveness. We also introduce the partial enumeration technique, which is designed to reduce the number of non-proper patterns in the solution space of the dynamic program. This technique helps to strengthen the lower bounds obtained by column generation and improve the quality of solutions found by the diving heuristic. Computational results are reported and compared on classical benchmarks from the literature as well as on new instances inspired from industrial data. According to these results, proposed diving algorithms outperform constructive and evolutionary heuristics.

## 7.11. On sets avoiding distance 1

In a joint work with C. Bachoc, T. Bellitto and P. Moustrou [39], 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  $4 \le \chi \left( G_{||.||_E} \right) \le 7$  (Nelson, Isbell 1950). The *measurable* chromatic number  $\chi_m$  of the graph  $G_{||.||}$  is the minimal number of *measurable* stable sets of  $G_{||.||}$  needed to cover all its vertices. Obviously, we have  $\chi \left( G_{||.||_E} \right) \le \chi_m \left( G_{||.||_E} \right)$ . For  $n = 2, 5 \le \chi_m \left( G_{||.||_E} \right)$  (Falconer 1981).

Let  $m_1(G_{||.||})$  denote the maximum density of a measurable set avoiding distance 1. We have  $\frac{1}{m_1(G_{||.||})} \leq \chi_m(G_{||.||})$ . 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  $\mathbb{R}^n$ ,  $||x||_P$  is the smallest positive real t such that  $x \in tP$ . Polytope norms include some usual norms such as the  $L^1$  and  $L^\infty$  norms.

If P tiles the space by translation, then it is easy to see that  $m_1(G_{||.||_P}) \ge \frac{1}{2^n}$ . 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.

## 7.12. Separating Codes and Traffic Monitoring

The paper [12] studies the problem of traffic monitoring which consists of differentiating a set of walks on a directed graph by placing sensors on as few arcs as possible. The problem of characterising a set of individuals by testing as few attributes as possible is already well-known, but traffic monitoring presents new challenges that the previous models of separation fall short from modelling such as taking into account the multiplicity and order of the arcs in a walk. We introduce a new and stronger model of separation based on languages that generalises the traffic monitoring problem. We study three subproblems with practical applications and develop methods to solve them by combining integer linear programming, separating codes and language theory.

## **SELECT Project-Team**

## 6. New Results

## 6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, 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 recently submitted an article where variables are sorted 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.

## **6.2.** Estimator selection and statistical tests

Participants: Sylvain Arlot, Matthieu Lerasle.

G. Maillard, S. Arlot and M. Lerasle studied a method mixing cross-validation with aggregation, called aggregated hold-out (Agghoo), which is already used by several practitioners. Agghoo can also be related to bagging. According to numerical experiments, Agghoo can improve significantly cross-validation's prediction error, at the same computational cost; this makes it very promising as a general-purpose tool for prediction. This work provides the first theoretical guarantees on Agghoo, in the supervised classification setting, ensuring that one can use it safely: at worst, Agghoo performs like hold-out, up to a constant factor. A non-asymptotic oracle inequality is also proved, in binary classification under the margin condition, which is sharp enough to get (fast) minimax rates.

With G. Lecué, Matthieu Lerasle working on "learning from MOM's principles", showing that a recent procedure by Lugosi and Mendelson can be derived by applying Le Cam's "estimation from tests" procedure to MOM's tests. They also showed some robustness properties of these estimators, proving that the rates of convergence of this estimator are not downgraded even if some "outliers" have corrupted the dataset, and the other data have only first and second moments equal to that of the targeted probability distribution.

## 6.3. Statistical learning methodology and theory

**Participants:** Gilles Celeux, Serge Cohen, Christine Keribin, Michel Prenat, Kaniav Kamary, Sylvain Arlot, Benjamin Auder, Jean-Michel Poggi, Neska El Haouij, Kevin Bleakley, Matthieu Lerasle.

Gilles Celeux and Serge Cohen have started research in collaboration with Agnès Grimaud (UVSQ) to perform clustering of hyperspectral images which respects spatial constraints. This is a one-class classification problem where distances between spectral images are given by the  $\chi^2$  distance, while spatial homogeneity is associated with a single link distance.

Gilles Celeux continued his collaboration with Jean-Patrick Baudry on model-based clustering. This year, they started work on assessing model-based clustering methods on cytometry data sets. The interest of these is that they involve combining clustering and classification tasks in a unified framework.

Gillies Celeux and Julie Josse have started research on missing data for model-based clustering in collaboration with Christophe Biernacki (Modal, Inria Lille). This year, they have proposed a model for mixture analysis involving not missing-at-random mixtures.

In the framework of MASSICCC, Benjamin Auder and Gilles Celeux have started research on the graphical representation of model-based clusters. The aim of this is to better-display proximity between clusters.

For a long time unsolved, the consistency and asymptotic normality of the maximum likelihood and variational estimators of the latent block model were finally tackled and obtained in a joint work with V. Brault and M. Mariadassou.

J-M. Poggi (with R. Genuer, C. Tuleau-Malot, N. Villa-Vialaneix), have published an article 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 Databootstrap and MapReduce respectively were tested on two massive datasets, one simulated one, and the other, real-world data.

With G. Lecué, Matthieu Lerasle worked on robust machine learning by median-of-means, providing an alternative to the Lugosi and Mendelson approach based on median of means for learning. This alternative is easier to present and to analyse theoretically. Furthermore, they proposed an algorithm to approximate this estimator, which could not be done for Lugosi and Mendelson's champions of tournaments (submitted).

## 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. Moreover, warranty cost calculations are made in the context of heterogeneous usages. This required estimations of mixtures and competing risk models in a highly-censored setting.

This year, Patrick Pamphile and Florence Ducros have published an article which proposes a two-component Weibull mixture model for modelling unobserved heterogeneity in heavily censored lifetime data collection. Performance of classical estimation methods (maximum of likelihood, EM, full Bayes and MCMC) are poor due to the high number of parameters and the heavy censoring. Thus, a Bayesian bootstrap method called Bayesian Restoration Maximization, was used. Sampling from the posterior distribution was obtained thanks to an importance sampling technique. Simulation results showed that, even with heavy censoring, BRM is effective both in term of estimate's precision and computation times.

## 6.6. Statistical analysis of genomic data

Participants: Gilles Celeux, 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), was 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 was available. They reduced the dimension of the network to avoid high-dimensional difficulties. Representing this network with a Gaussian graphical model, the following procedure was 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 collaboration with Benno Schwikowski, Iryna Nikolayeva and Anavaj Sakuntabhai (Pasteur Institute, Paris), Kevin Bleakley worked 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, and an article has now been submitted.

In collaboration with researchers from the Pasteur Institute, Kevin Bleakley worked on statistical tests in the context of research into what leads to dengue fever *without symptoms* as opposed to *with* symptoms. This work was published in *Science Translational Medicine*.

Kevin Bleakley has also collaborated with Inserm/Paris-Saclay researchers at Kremlin-Bicêtre hospital on cyclic transcriptional clocks and renal corticosteroid signaling, and has developed novel statistical tests for detecting synchronous signals. This work is submitted.

## 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 worked on the detection of associations between drugs and adverse events in the framework of the PhD of Valerie Robert, which was defended this year. At first, this team developed model-based clustering inspired by latent block models (LBMs), which consists of co-clustering rows and columns of two binary tables, imposing the same row ranking. This enabled 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 demonstrated the interest of the proposed model, compared with standard contingency table analysis, to detect co-prescription and masking effects.

Futhermore, with V. Robert, C. Kerebin and G. Celeux showed that it can be useful to use an LBM model on a contingency table of drugs and adverse effects to do cluster initialization for dealing with individual's data.

## 6.8. Statistical rating and ranking of scientific journals

Participants: Gilles Celeux, Julie Josse, Jean-Louis Foulley.

In collaboration with Jean-Louis Foulley (Montpellier University), Gilles Celeux and Julie Josse have done research on the statistical rating and ranking of scientific journals. They have proposed Dirichlet multinomial Bayesian models for pagerank-type algorithms allowing self-citations to be excluded. The resulting methods were tested on a set of 47 scientific journals.

## 6.9. Statistical mathematics

Participant: Matthieu Lerasle.

In collaboration with R. Diel, Matthieu Lerasle published an article on nonparametric estimation for random walks in random environments. They proposed a non-parametric approach for estimating the distribution of the environment from the observation of one trajectory of a random walk in it. They obtained risk bounds in sup-norm for the cumulative distribution function of the environment.

## 6.10. Random graph theory

Participant: Matthieu Lerasle.

In collaboration with R. Chetrite and R. Diel, Matthieu Lerasle published an article on the number of potential winners in the Bradley-Terry model in random environments. They proposed the first mathematical study of the Bradley-Terry model where the values of players are i.i.d. realisations of some distribution. They proved that a Bradley-Terry tournament is fair (in the sense that the best player ends up with the largest number of victories) under a certain convexity condition on the tail distribution of the values. They also showed that this condition is sharp and provided sharp estimate of the number of potential winners when the condition fails.

He also collaborated with R. Diel and S. Le Corff on learning latent structures of large random graphs, investigating the possibility of estimating latent structure in sparsely observed random graphs. The main example was a Bradley-Terry tournament where each team has only played a few games. It is well known that individual values of the teams cannot be consistently estimated in this setting. They showed that their distribution on the other hand can be, and provide general tools for bounding the risk of the maximum likelihood estimator (submitted).

## **SEQUEL Project-Team**

## 7. New Results

## 7.1. Decision-making Under Uncertainty

### 7.1.1. Reinforcement Learning

#### Thompson Sampling for Linear-Quadratic Control Problems, [22]

We consider the exploration-exploitation tradeoff in linear quadratic (LQ) control problems, where the state dynamics is linear and the cost function is quadratic in states and controls. We analyze the regret of Thompson sampling (TS) (a.k.a. posterior-sampling for reinforcement learning) in the frequentist setting, i.e., when the parameters characterizing the LQ dynamics are fixed. Despite the empirical and theoretical success in a wide range of problems from multi-armed bandit to linear bandit, we show that when studying the frequentist regret TS in control problems, we need to trade-off the frequency of sampling optimistic parameters and the frequency of switches in the control policy. This results in an overall regret of  $O(T^{2/3})$ , which is significantly worse than the regret  $O(\sqrt{T})$  achieved by the optimism-in-face-of-uncertainty algorithm in LQ control problems.

#### Exploration-Exploitation in MDPs with Options, [33]

While a large body of empirical results show that temporally-extended actions and options may significantly affect the learning performance of an agent, the theoretical understanding of how and when options can be beneficial in online reinforcement learning is relatively limited. In this paper, we derive an upper and lower bound on the regret of a variant of UCRL using options. While we first analyze the algorithm in the general case of semi-Markov decision processes (SMDPs), we show how these results can be translated to the specific case of MDPs with options and we illustrate simple scenarios in which the regret of learning with options can be provably much smaller than the regret suffered when learning with primitive actions.

#### Regret Minimization in MDPs with Options without Prior Knowledge, [34]

The option framework integrates temporal abstraction into the reinforcement learning model through the introduction of macro-actions (i.e., options). Recent works leveraged the mapping of Markov decision processes (MDPs) with options to semi-MDPs (SMDPs) and introduced SMDP-versions of exploration-exploitation algorithms (e.g., RMAX-SMDP and UCRL-SMDP) to analyze the impact of options on the learning performance. Nonetheless, the PAC-SMDP sample complexity of RMAX-SMDP can hardly be translated into equivalent PAC-MDP theoretical guarantees, while the regret analysis of UCRL-SMDP requires prior knowledge of the distributions of the cumulative reward and duration of each option, which are hardly available in practice. In this paper, we remove this limitation by combining the SMDP view together with the inner Markov structure of options into a novel algorithm whose regret performance matches UCRL-SMDP's up to an additive regret term. We show scenarios where this term is negligible and the advantage of temporal abstraction is preserved. We also report preliminary empirical results supporting the theoretical findings.

#### Is the Bellman Residual a Bad Proxy?, [36]

This paper aims at theoretically and empirically comparing two standard optimization criteria for Reinforcement Learning: i) maximization of the mean value and ii) minimization of the Bellman residual. For that purpose, we place ourselves in the framework of policy search algorithms, that are usually designed to maximize the mean value, and derive a method that minimizes the residual T \* v  $\pi$  – v  $\pi$  1, $\nu$  over policies. A theoretical analysis shows how good this proxy is to policy optimization , and notably that it is better than its value-based counterpart. We also propose experiments on randomly generated generic Markov decision processes, specifically designed for studying the influence of the involved concentrability coefficient. They show that the Bellman residual is generally a bad proxy to policy optimization and that directly maximizing the mean value is much better, despite the current lack of deep theoretical analysis. This might seem obvious, as directly addressing the problem of interest is usually better, but given the prevalence of (projected) Bellman residual minimization in value-based reinforcement learning, we believe that this question is worth to be considered.

#### Faut-il minimiser le résidu de Bellman ou maximiser la valeur moyenne ?, [56]

#### Transfer Reinforcement Learning with Shared Dynamics, [38]

This article addresses a particular Transfer Reinforcement Learning (RL) problem: when dynamics do not change from one task to another, and only the reward function does. Our method relies on two ideas, the first one is that transition samples obtained from a task can be reused to learn on any other task: an immediate reward estimator is learnt in a supervised fashion and for each sample, the reward entry is changed by its reward estimate. The second idea consists in adopting the optimism in the face of uncertainty principle and to use upper bound reward estimates. Our method is tested on a navigation task, under four Transfer RL experimental settings: with a known reward function, with strong and weak expert knowledge on the reward function, and with a completely unknown reward function. It is also evaluated in a Multi-Task RL experiment and compared with the state-of-the-art algorithms. Results reveal that this method constitutes a major improvement for transfer/multi-task problems that share dynamics.

#### 7.1.2. Multi-arm Bandit Theory

#### Trading Off Rewards and Errors in Multi-armed Bandits, [31]

In multi-armed bandits, the most common objective is the maximization of the cumulative reward. Alternative settings include active exploration, where a learner tries to gain accurate estimates of the rewards of all arms. While these objectives are contrasting, in many scenarios it is desirable to trade off rewards and errors. For instance, in educational games the designer wants to gather generalizable knowledge about the behavior of the students and teaching strategies (small estimation errors) but, at the same time, the system needs to avoid giving a bad experience to the players, who may leave the system permanently (large reward). In this paper, we formalize this tradeoff and introduce the ForcingBalance algorithm whose performance is provably close to the best possible tradeoff strategy. Finally, we demonstrate on real-world educational data that ForcingBalance returns useful information about the arms without compromising the overall reward.

#### Online Influence Maximization Under Independent Cascade Model with Semi-bandit Feedback, [54]

We study the online influence maximization problem in social networks under the independent cascade model. Specifically, we aim to learn the set of "best influencers " in a social network online while repeatedly interacting with it. We address the challenges of (i) combinatorial action space, since the number of feasible influencer sets grows exponentially with the maximum number of influencers, and (ii) limited feedback, since only the influenced portion of the network is observed. Under a stochastic semi-bandit feedback, we propose and analyze IMLinUCB, a computationally efficient UCB-based algorithm. Our bounds on the cumulative regret are polynomial in all quantities of interest, achieve near-optimal dependence on the number of interactions and reflect the topology of the network and the activation probabilities of its edges, thereby giving insights on the problem complexity. To the best of our knowledge, these are the first such results. Our experiments show that in several representative graph topologies, the regret of IMLinUCB scales as suggested by our upper bounds. IMLinUCB permits linear generalization and thus is both statistically and computationally suitable for large-scale problems. Our experiments also show that IMLinUCB with linear generalization can lead to low regret in real-world online influence maximization.

#### Boundary Crossing for General Exponential Families, [39]

We consider parametric exponential families of dimension K on the real line. We study a variant of boundary crossing probabilities coming from the multi-armed bandit literature, in the case when the real-valued distributions form an exponential family of dimension K. Formally, our result is a concentration inequality that bounds the probability that B  $\psi$  ( $\theta$  n ,  $\theta$ ) f (t/n)/n, where  $\theta$  is the parameter of an unknown target distribution,  $\theta$  n is the empirical parameter estimate built from n observations,  $\psi$  is the log-partition function of the exponential family and B  $\psi$  is the corresponding Bregman divergence. From the perspective of stochastic multi-armed bandits, we pay special attention to the case when the boundary function f is logarithmic, as it enables to

analyze the regret of the state-of-the-art KL-ucb and KL-ucb+ strategies, whose analysis was left open in such generality. Indeed, previous results only hold for the case when K = 1, while we provide results for arbitrary finite dimension K, thus considerably extending the existing results. Perhaps surprisingly, we highlight that the proof techniques to achieve these strong results already existed three decades ago in the work of T.L. Lai, and were apparently forgotten in the bandit community. We provide a modern rewriting of these beautiful techniques that we believe are useful beyond the application to stochastic multi-armed bandits.

#### The Non-stationary Stochastic Multi-armed Bandit Problem, Robin, Féraud, Maillard [64]<sup>0</sup>

#### Linear Thompson Sampling Revisited, [21]

We derive an alternative proof for the regret of Thompson sampling (TS) in the stochastic linear bandit setting. While we obtain a regret bound of order  $\tilde{O}(d^{3/2}\sqrt{T})$  as in previous results, the proof sheds new light on the functioning of the TS. We leverage on the structure of the problem to show how the regret is related to the sensitivity (i.e., the gradient) of the objective function and how selecting optimal arms associated to *optimistic* parameters does control it. Thus we show that TS can be seen as a generic randomized algorithm where the sampling distribution is designed to have a fixed probability of being optimistic, at the cost of an additional  $\sqrt{d}$  regret factor compared to a UCB-like approach. Furthermore, we show that our proof can be readily applied to regularized linear optimization and generalized linear model problems.

#### Active Learning for Accurate Estimation of Linear Models, [47]

We explore the sequential decision-making problem where the goal is to estimate a number of linear models uniformly well, given a shared budget of random contexts independently sampled from a known distribution. For each incoming context, the decision-maker selects one of the linear models and receives an observation that is corrupted by the unknown noise level of that model. We present Trace-UCB, an adaptive allocation algorithm that learns the models' noise levels while balancing contexts accordingly across them, and prove bounds for its simple regret in both expectation and high-probability. We extend the algorithm and its bounds to the high dimensional setting , where the number of linear models times the dimension of the contexts is more than the total budget of samples. Simulations with real data suggest that Trace-UCB is remarkably robust , outperforming a number of baselines even when its assumptions are violated.

#### Learning the Distribution with Largest Mean: Two Bandit Frameworks, [18]

Over the past few years, the multi-armed bandit model has become increasingly popular in the machine learning community, partly because of applications including online content optimization. This paper reviews two different sequential learning tasks that have been considered in the bandit literature ; they can be formulated as (sequentially) learning which distribution has the highest mean among a set of distributions, with some constraints on the learning process. For both of them (regret minimization and best arm identification) we present recent, asymptotically optimal algorithms. We compare the behaviors of the sampling rule of each algorithm as well as the complexity terms associated to each problem.

#### On Bayesian Index Policies for Sequential Resource Allocation, [19]

This paper is about index policies for minimizing (frequentist) regret in a stochastic multi-armed bandit model, inspired by a Bayesian view on the problem. Our main contribution is to prove that the Bayes-UCB algorithm, which relies on quantiles of posterior distributions, is asymptotically optimal when the reward distributions belong to a one-dimensional exponential family, for a large class of prior distributions. We also show that the Bayesian literature gives new insight on what kind of exploration rates could be used in frequentist, UCB-type algorithms. Indeed, approximations of the Bayesian optimal solution or the Finite Horizon Gittins indices provide a justification for the kl-UCB+ and kl-UCB-H+ algorithms, whose asymptotic optimality is also established.

#### Multi-Player Bandits Models Revisited, [59]

Multi-player Multi-Armed Bandits (MAB) have been extensively studied in the literature, motivated by applications to Cognitive Radio systems. Driven by such applications as well, we motivate the introduction

<sup>&</sup>lt;sup>0</sup>This work has been done while OA. Maillard was at Inria Saclay, in the TAO team.

of several levels of feedback for multi-player MAB algorithms. Most existing work assume that sensing information is available to the algorithm. Under this assumption, we improve the state-of-the-art lower bound for the regret of any decentralized algorithms and introduce two algorithms, RandTopM and MCTopM, that are shown to empirically outperform existing algorithms. Moreover, we provide strong theoretical guarantees for these algorithms, including a notion of asymptotic optimality in terms of the number of selections of bad arms. We then introduce a promising heuristic, called Selfish, that can operate without sensing information, which is crucial for emerging applications to Internet of Things networks. We investigate the empirical performance of this algorithm and provide some first theoretical elements for the understanding of its behavior.

#### Multi-Armed Bandit Learning in IoT Networks: Learning helps even in non-stationary settings, [57]

Setting up the future Internet of Things (IoT) networks will require to support more and more communicating devices. We prove that intelligent devices in unlicensed bands can use Multi-Armed Bandit (MAB) learning algorithms to improve resource exploitation. We evaluate the performance of two classical MAB learning algorithms, UCB1 and Thompson Sampling, to handle the decentralized decision-making of Spectrum Access, applied to IoT networks; as well as learning performance with a growing number of intelligent end-devices. We show that using learning algorithms does help to fit more devices in such networks, even when all end-devices are intelligent and are dynamically changing channel. In the studied scenario, stochastic MAB learning provides a up to 16% gain in term of successful transmission probabilities, and has near optimal performance even in non-stationary and non-i.i.d. settings with a majority of intelligent devices.

#### 7.1.3. Nonparametric Statistics of Time Series

#### Efficient Tracking of a Growing Number of Experts, [41]

We consider a variation on the problem of prediction with expert advice, where new forecasters that were unknown until then may appear at each round. As often in prediction with expert advice, designing an algorithm that achieves near-optimal regret guarantees is straightforward, using aggregation of experts. However, when the comparison class is sufficiently rich, for instance when the best expert and the set of experts itself changes over time, such strategies naively require to maintain a prohibitive number of weights (typically exponential with the time horizon). By contrast, designing strategies that both achieve a near-optimal regret and maintain a reasonable number of weights is highly non-trivial. We consider three increasingly challenging objectives (simple regret, shifting regret and sparse shifting regret) that extend existing notions defined for a fixed expert ensemble; in each case, we design strategies that achieve tight regret bounds, adaptive to the parameters of the comparison class, while being computationally inexpensive. Moreover, our algorithms are anytime, agnostic to the number of incoming experts and completely parameter-free. Such remarkable results are made possible thanks to two simple but highly effective recipes: first the " abstention trick " that comes from the specialist framework and enables to handle the least challenging notions of regret, but is limited when addressing more sophisticated objectives. Second, the "muting trick" that we introduce to give more flexibility. We show how to combine these two tricks in order to handle the most challenging class of comparison strategies.

#### 7.1.4. Stochastic Games

#### Monte-Carlo Tree Search by Best Arm Identification, [37]

Recent advances in bandit tools and techniques for sequential learning are steadily enabling new applications and are promising the resolution of a range of challenging related problems. We study the game tree search problem, where the goal is to quickly identify the optimal move in a given game tree by sequentially sampling its stochastic payoffs. We develop new algorithms for trees of arbitrary depth, that operate by summarizing all deeper levels of the tree into confidence intervals at depth one, and applying a best arm identification procedure at the root. We prove new sample complexity guarantees with a refined dependence on the problem instance. We show experimentally that our algorithms outperform existing elimination-based algorithms and match previous special-purpose methods for depth-two trees.

#### Learning Nash Equilibrium for General-Sum Markov Games from Batch Data, [46]

This paper addresses the problem of learning a Nash equilibrium in  $\gamma$ -discounted mul-tiplayer general-sum Markov Games (MGs) in a batch setting. As the number of players increases in MG, the agents may either collaborate or team apart to increase their final rewards. One solution to address this problem is to look for a Nash equilibrium. Although , several techniques were found for the subcase of two-player zero-sum MGs, those techniques fail to find a Nash equilibrium in general-sum Markov Games. In this paper, we introduce a new definition of-Nash equilibrium in MGs which grasps the strategy's quality for multiplayer games. We prove that minimizing the norm of two Bellman-like residuals implies to learn such an-Nash equilibrium. Then, we show that minimizing an empirical estimate of the L p norm of these Bellman-like residuals allows learning for general-sum games within the batch setting. Finally, we introduce a neural network architecture that successfully learns a Nash equilibrium in generic multiplayer general-sum turn-based MGs.

#### 7.1.5. Automata Learning

#### Spectral Learning from a Single Trajectory under Finite-State Policies, [23]

We present spectral methods of moments for learning sequential models from a single trajectory, in stark contrast with the classical literature that assumes the availability of multiple i.i.d. trajectories. Our approach leverages an efficient SVD-based learning algorithm for weighted automata and provides the first rigorous analysis for learning many important models using dependent data. We state and analyze the algorithm under three increasingly difficult scenarios: probabilistic automata, stochastic weighted automata, and reactive predictive state representations controlled by a finite-state policy. Our proofs include novel tools for studying mixing properties of stochastic weighted automata.

### 7.1.6. Online Kernel and Graph-Based Methods

#### Distributed Adaptive Sampling for Kernel Matrix Approximation, [26]

Most kernel-based methods, such as kernel regression, kernel PCA, ICA, or k-means clustering, do not scale to large datasets, because constructing and storing the kernel matrix  $\mathbf{K}_n$  requires at least  $O(n^2)$  time and space for *n* samples. Recent works (Alaoui 2014, Musco 2016) show that sampling points with replacement according to their ridge leverage scores (RLS) generates small dictionaries of relevant points with strong spectral approximation guarantees for  $\mathbf{K}_n$ . The drawback of RLS-based methods is that computing exact RLS requires constructing and storing the whole kernel matrix. In this paper, we introduce SQUEAK, a new algorithm for kernel approximation based on RLS sampling that sequentially processes the dataset, storing a dictionary which creates accurate kernel matrix approximations with a number of points that only depends on the effective dimension  $d_{\text{eff}}(\gamma)$  of the dataset. Moreover since all the RLS estimations are efficiently performed using only the small dictionary, SQUEAK never constructs the whole matrix  $\mathbf{K}_n$  runs in linear time  $\widetilde{O}(nd_{\text{eff}}(\gamma)^3)$  w.r.t. *n*, and requires only a single pass over the dataset. We also propose a parallel and distributed version of SQUEAK achieving similar accuracy in as little as  $\widetilde{O}(log(n)d_{\text{eff}}(\gamma)^3)$  time.

#### Second-Order Kernel Online Convex Optimization with Adaptive Sketching, [28]

Kernel online convex optimization (KOCO) is a framework combining the expressiveness of non-parametric kernel models with the regret guarantees of online learning. First-order KOCO methods such as functional gradient descent require only O(t) time and space per iteration, and, when the only information on the losses is their convexity, achieve a minimax optimal  $O(\sqrt{T})$  regret. Nonetheless, many common losses in kernel problems, such as squared loss, logistic loss, and squared hinge loss posses stronger curvature that can be exploited. In this case, second-order KOCO methods achieve  $O(\log(Det(K)))$  regret, which we show scales as  $O(d_{eff} \log T)$ , where  $d_{eff}$  is the effective dimension of the problem and is usually much smaller than  $O(\sqrt{T})$ . The main drawback of second-order methods is their much higher  $O(t^2)$  space and time complexity. In this paper, we introduce kernel online Newton step (KONS), a new second-order KOCO methods, we introduce a new matrix sketching algorithm for the kernel matrix K, and show that for a chosen parameter  $\gamma \leq 1$  our Sketched-KONS reduces the space and time complexity by a factor of  $\gamma^2$  to  $O(t^2\gamma^2)$  space and time per iteration, while incurring only  $1/\gamma$  times more regret.

#### Efficient Second-order Online Kernel Learning with Adaptive Embedding, [27]

Online kernel learning (OKL) is a flexible framework to approach prediction problems, since the large approximation space provided by reproducing kernel Hilbert spaces can contain an accurate function for the problem. Nonetheless, optimizing over this space is computationally expensive. Not only first order methods accumulate  $O(\sqrt{T})$  more loss than the optimal function, but the curse of kernelization results in a O(t) per step complexity. Second-order methods get closer to the optimum much faster, suffering only  $O(\log(T))$  regret, but second-order updates are even more expensive, with a  $O(t^2)$  per-step cost. Existing approximate OKL methods try to reduce this complexity either by limiting the Support Vectors (SV) introduced in the predictor, or by avoiding the kernelization process altogether using embedding. Nonetheless, as long as the size of the approximation space or the number of SV does not grow over time, an adversary can always exploit the approximation process. In this paper, we propose PROS-N-KONS, a method that combines Nystrom sketching to project the input point in a small, accurate embedded space, and performs efficient second-order updates in this space. The embedded space is continuously updated to guarantee that the embedding remains accurate, and we show that the per-step cost only grows with the effective dimension of the problem and not with T. Moreover, the second-order updated allows us to achieve the logarithmic regret. We empirically compare our algorithm on recent large-scales benchmarks and show it performs favorably.

#### Zonotope Hit-and-run for Efficient Sampling from Projection DPPs, [35]

Determinantal point processes (DPPs) are distributions over sets of items that model diversity using kernels. Their applications in machine learning include summary extraction and recommendation systems. Yet, the cost of sampling from a DPP is prohibitive in large-scale applications, which has triggered an effort towards efficient approximate samplers. We build a novel MCMC sampler that combines ideas from combinatorial geometry, linear programming, and Monte Carlo methods to sample from DPPs with a fixed sample cardinality, also called projection DPPs. Our sampler leverages the ability of the hit-and-run MCMC kernel to efficiently move across convex bodies. Previous theoretical results yield a fast mixing time of our chain when targeting a distribution that is close to a projection DPP, but not a DPP in general. Our empirical results demonstrate that this extends to sampling projection DPPs, i.e., our sampler is more sample-efficient than previous approaches which in turn translates to faster convergence when dealing with costly-to-evaluate functions, such as summary extraction in our experiments.

## 7.2. Statistical Learning and Bayesian Analysis

#### Universality of Bayesian mixture predictors, [50]

The problem is that of sequential probability forecasting for finite-valued time series. The data is generated by an unknown probability distribution over the space of all one-way infinite sequences. It is known that this measure belongs to a given set C, but the latter is completely arbitrary (uncountably infinite, without any structure given). The performance is measured with asymptotic average log loss. In this work it is shown that the minimax asymptotic performance is always attainable, and it is attained by a convex combination of a countably many measures from the set C (a Bayesian mixture). This was previously only known for the case when the best achievable asymptotic error is 0. This also contrasts previous results that show that in the nonrealizable case all Bayesian mixtures may be suboptimal, while there is a predictor that achieves the optimal performance.

#### Hypotheses Testing on Infinite Random Graphs, [48]

Drawing on some recent results that provide the formalism necessary to definite stationarity for infinite random graphs, this paper initiates the study of statistical and learning questions pertaining to these objects. Specifically, a criterion for the existence of a consistent test for complex hypotheses is presented, generalizing the corresponding results on time series. As an application, it is shown how one can test that a tree has the Markov property, or,more generally, to estimate its memory.

#### Independence Clustering (Without a Matrix), [49]

The independence clustering problem is considered in the following formulation: given a set S of random variables, it is required to find the finest partitioning  $\{U_1, \dots, U_k\}$  of S into clusters such that the clusters  $U_1, \dots, U_k$  are mutually independent. Since mutual independence is the target, pairwise similarity

measurements are of no use, and thus traditional clustering algorithms are inapplicable. The distribution of the random variables in S is, in general, unknown, but a sample is available. Thus, the problem is cast in terms of time series. Two forms of sampling are considered: i.i.d. and stationary time series, with the main emphasis being on the latter, more general, case. A consistent, computationally tractable algorithm for each of the settings is proposed, and a number of open directions for further research are outlined.

## 7.3. Applications

### 7.3.1. Dialogue Systems and Natural Language

#### End-to-end Optimization of Goal-driven and Visually Grounded Dialogue Systems, [51]

End-to-end design of dialogue systems has recently become a popular research topic thanks to powerful tools such as encoder-decoder architectures for sequence-to-sequence learning. Yet, most current approaches cast human-machine dialogue management as a supervised learning problem, aiming at predicting the next utterance of a participant given the full history of the dialogue. This vision is too simplistic to render the intrinsic planning problem inherent to dialogue as well as its grounded nature , making the context of a dialogue larger than the sole history. This is why only chitchat and question answering tasks have been addressed so far using end-to-end architectures. In this paper, we introduce a Deep Reinforcement Learning method to optimize visually grounded task-oriented dialogues , based on the policy gradient algorithm. This approach is tested on a dataset of 120k dialogues collected through Mechanical Turk and provides encouraging results at solving both the problem of generating natural dialogues and the task of discovering a specific object in a complex picture.

#### Online Learning and Transfer for User Adaptation in Dialogue Systems, [58]

We address the problem of user adaptation in Spoken Dialogue Systems. The goal is to quickly adapt online to a new user given a large amount of dialogues collected with other users. Previous works using Transfer for Reinforcement Learning tackled this problem when the number of source users remains limited. In this paper, we overcome this constraint by clustering the source users: each user cluster, represented by its centroid, is used as a potential source in the state-of-the-art Transfer Reinforcement Learning algorithm. Our benchmark compares several clustering approaches , including one based on a novel metric. All experiments are led on a negotiation dialogue task, and their results show significant improvements over baselines.

#### GuessWhat?! Visual Object Discovery Through Multi-modal Dialogue, [29]

We introduce GuessWhat?!, a two-player guessing game as a testbed for research on the interplay of computer vision and dialogue systems. The goal of the game is to locate an unknown object in a rich image scene by asking a sequence of questions. Higher-level image understanding, like spatial reasoning and language grounding, is required to solve the proposed task. Our key contribution is the collection of a large-scale dataset consisting of 150K human-played games with a total of 800K visual question-answer pairs on 66K images. We explain our design decisions in collecting the dataset and introduce the oracle and questioner tasks that are associated with the two players of the game. We prototyped deep learning models to establish initial base-lines of the introduced tasks.

#### LIG-CRIStAL System for the WMT17 Automatic Post-Editing Task, [25]

This paper presents the LIG-CRIStAL submission to the shared Automatic Post-Editing task of WMT 2017. We propose two neural post-editing models: a mono-source model with a task-specific attention mechanism, which performs particularly well in a low-resource scenario; and a chained architecture which makes use of the source sentence to provide extra context. This latter architecture manages to slightly improve our results when more training data is available. We present and discuss our results on two datasets (en-de and de-en) that are made available for the task.

### 7.3.2. Recommendation systems

A Multi-Armed Bandit Model Selection for Cold-Start User Recommendation, [32]

How can we effectively recommend items to a user about whom we have no information? This is the problem we focus on, known as the cold-start problem. In this paper, we focus on the cold user problem. In most existing works, the cold-start problem is handled through the use of many kinds of information available about the user. However, what happens if we do not have any information? Recommender systems usually keep a substantial amount of prediction models that are available for analysis. Moreover, recommendations to new users yield uncertain returns. Assuming a number of alternative prediction models is available to select items to recommend to a cold user, this paper introduces a multi-armed bandit based model selection, named PdMS.In comparison with two baselines, PdMS improves the performance as measured by the nDCG. These improvements are demonstrated on real, public datasets.

#### 7.3.3. Software development

#### A Large-scale Study of Call Graph-based Impact Prediction using Mutation Testing, [20]

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.

#### Correctness Attraction: A Study of Stability of Software Behavior under Runtime Perturbation, [15]

Can the execution of a software be perturbed without breaking the correctness of the output? In this paper, we devise a novel protocol to answer this rarely investigated question. In an experimental study, we observe that many perturbations do not break the correctness in ten subject programs. We call this phenomenon "correctness attraction". The uniqueness of this protocol is that it considers a systematic exploration of the perturbation space as well as perfect oracles to determine the correctness of the output. To this extent, our findings on the stability of software under execution perturbations have a level of validity that has never been reported before in the scarce related work. A qualitative manual analysis enables us to set up the first taxonomy ever of the reasons behind correctness attraction.

#### 7.3.4. Graph theory

#### A generative model for sparse, evolving digraphs, [43]

Generating graphs that are similar to real ones is an open problem, while the similarity notion is quite elusive and hard to formalize. In this paper, we focus on sparse digraphs and propose SDG, an algorithm that aims at generating graphs similar to real ones. Since real graphs are evolving and this evolution is important to study in order to understand the underlying dynamical system, we tackle the problem of generating series of graphs. We propose SEDGE, an algorithm meant to generate series of graphs similar to a real series. SEDGE is an extension of SDG. We consider graphs that are representations of software programs and show experimentally that our approach outperforms other existing approaches. Experiments show the performance of both algorithms.

## A Spectral Algorithm with Additive Clustering for the Recovery of Overlapping Communities in Networks, [17]

This paper presents a novel spectral algorithm with additive clustering designed to identify overlapping communities in networks. The algorithm is based on geometric properties of the spectrum of the expected adjacency matrix in a random graph model that we call stochastic blockmodel with overlap (SBMO). An adaptive version of the algorithm, that does not require the knowledge of the number of hidden communities, is proved to be consistent under the SBMO when the degrees in the graph are (slightly more than) logarithmic. The algorithm is shown to perform well on simulated data and on real-world graphs with known overlapping communities.

#### 7.3.5. Deep Learning

#### Modulating early visual processing by language, [30]

It is commonly assumed that language refers to high-level visual concepts while leaving low-level visual processing unaffected. This view dominates the current literature in computational models for language-vision tasks, where visual and linguistic inputs are mostly processed independently before being fused into a single representation. In this paper, we deviate from this classic pipeline and propose to modulate the entire visual processing by a linguistic input. Specifically, we introduce Conditional Batch Normalization (CBN) as an efficient mechanism to modulate convolutional feature maps by a linguistic embedding. We apply CBN to a pre-trained Residual Network (ResNet), leading to the MODulatEd ResNet (MODERN) architecture, and show that this significantly improves strong baselines on two visual question answering tasks. Our ablation study confirms that modulating from the early stages of the visual processing is beneficial.

#### FiLM: Visual Reasoning with a General Conditioning Layer, [45]

We introduce a general-purpose conditioning method for neural networks called FiLM: Feature-wise Linear Modulation. FiLM layers influence neural network computation via a simple , feature-wise affine transformation based on conditioning information. We show that FiLM layers are highly effective for visual reasoning - answering image-related questions which require a multi-step, high-level process - a task which has proven difficult for standard deep learning methods that do not explicitly model reasoning. Specifically, we show on visual reasoning tasks that FiLM layers 1) halve state-of-the-art error for the CLEVR benchmark, 2) modulate features in a coherent manner, 3) are robust to ablations and architectural modifications, and 4) generalize well to challenging, new data from few examples or even zero-shot.

#### Learning Visual Reasoning Without Strong Priors, [44]

Achieving artificial visual reasoning - the ability to answer image-related questions which require a multistep, high-level process - is an important step towards artificial general intelligence. This multi-modal task requires learning a question-dependent, structured reasoning process over images from language. Standard deep learning approaches tend to exploit biases in the data rather than learn this underlying structure, while leading methods learn to visually reason successfully but are hand-crafted for reasoning. We show that a general-purpose, Conditional Batch Normalization approach achieves state-of-the-art results on the CLEVR Visual Reasoning benchmark with a 2.4% error rate. We outperform the next best end-to-end method (4.5%) and even methods that use extra supervision (3.1%). We probe our model to shed light on how it reasons, showing it has learned a question-dependent, multi-step process. Previous work has operated under the assumption that visual reasoning calls for a specialized architecture, but we show that a general architecture with proper conditioning can learn to visually reason effectively. Index Terms: Deep Learning, Language and Vision Note: A full paper extending this study is available at http: //arxiv.org/abs/1709.07871, with additional references , experiments, and analysis.

#### HoME: a Household Multimodal Environment, [24]

We introduce HoME: a Household Multimodal Environment for artificial agents to learn from vision, audio, semantics, physics, and interaction with objects and other agents, all within a realistic context. HoME integrates over 45,000 diverse 3D house layouts based on the SUNCG dataset, a scale which may facilitate learning, generalization, and transfer. HoME is an open-source, OpenAI Gym-compatible platform extensible to tasks in reinforcement learning, language grounding, sound-based navigation, robotics, multi-agent learning, and more. We hope HoME better enables artificial agents to learn as humans do: in an interactive, multimodal, and richly contextualized setting.

## **SIERRA Project-Team**

## 6. New Results

## 6.1. On Structured Prediction Theory with Calibrated Convex Surrogate Losses

In [16], we provide novel theoretical insights on structured prediction in the context of efficient convex surrogate loss minimization with consistency guarantees. For any task loss, we construct a convex surrogate that can be optimized via stochastic gradient descent and we prove tight bounds on the so-called "calibration function" relating the excess surrogate risk to the actual risk. In contrast to prior related work, we carefully monitor the effect of the exponential number of classes in the learning guarantees as well as on the optimization complexity. As an interesting consequence, we formalize the intuition that some task losses make learning harder than others, and that the classical 0-1 loss is ill-suited for general structured prediction.

## 6.2. Domain-Adversarial Training of Neural Networks

In [18], we introduce a new representation learning approach for domain adaptation, in which data at training and test time come from similar but different distributions. Our approach is directly inspired by the theory on domain adaptation suggesting that, for effective domain transfer to be achieved, predictions must be made based on features that cannot discriminate between the training (source) and test (target) domains. The approach implements this idea in the context of neural network architectures that are trained on labeled data from the source domain and unlabeled data from the target domain (no labeled target-domain data is necessary). As the training progresses, the approach promotes the emergence of features that are (i) discriminative for the main learning task on the source domain and (ii) indiscriminate with respect to the shift between the domains. We show that this adaptation behaviour can be achieved in almost any feed-forward model by augmenting it with few standard layers and a new gradient reversal layer. The resulting augmented architecture can be trained using standard backpropagation and stochastic gradient descent, and can thus be implemented with little effort using any of the deep learning packages. We demonstrate the success of our approach for two distinct classification problems (document sentiment analysis and image classification), where state-of-the-art domain adaptation performance on standard benchmarks is achieved. We also validate the approach for descriptor learning task in the context of person re-identification application.

# 6.3. Linearly Convergent Randomized Iterative Methods for Computing the Pseudoinverse

In [25], we develop the first stochastic incremental method for calculating the Moore-Penrose pseudoinverse of a real matrix. By leveraging three alternative characterizations of pseudoinverse matrices, we design three methods for calculating the pseudoinverse: two general purpose methods and one specialized to symmetric matrices. The two general purpose methods are proven to converge linearly to the pseudoinverse of any given matrix. For calculating the pseudoinverse of full rank matrices we present two additional specialized methods which enjoy a faster convergence rate than the general purpose methods. We also indicate how to develop randomized methods for calculating approximate range space projections, a much needed tool in inexact Newton type methods or quadratic solvers when linear constraints are present. Finally, we present numerical experiments of our general purpose methods for calculating pseudoinverses and show that our methods greatly outperform the Newton-Schulz method on large dimensional matrices.

# 6.4. Sharp asymptotic and finite-sample rates of convergence of empirical measures in Wasserstein distance

The Wasserstein distance between two probability measures on a metric space is a measure of closeness with applications in statistics, probability, and machine learning. In [39], we consider the fundamental question of how quickly the empirical measure obtained from n independent samples from  $\mu$  approaches  $\mu$  in the Wasserstein distance of any order. We prove sharp asymptotic and finite-sample results for this rate of convergence for general measures on general compact metric spaces. Our finite-sample results show the existence of multi-scale behavior, where measures can exhibit radically different rates of convergence as n grows. Collaboration with Jonathan Weed, Francis Bach)

## 6.5. Efficient Algorithms for Non-convex Isotonic Regression through Submodular Optimization

In [19], we consider the minimization of submodular functions subject to ordering constraints. We show that this optimization problem can be cast as a convex optimization problem on a space of uni-dimensional measures, with ordering constraints corresponding to first-order stochastic dominance. We propose new discretization schemes that lead to simple and efficient algorithms based on zero-th, first, or higher order oracles; these algorithms also lead to improvements without isotonic constraints. Finally, our experiments show that non-convex loss functions can be much more robust to outliers for isotonic regression, while still leading to an efficient optimization problem.

## 6.6. Bridging the Gap between Constant Step Size Stochastic Gradient Descent and Markov Chains

In [21], we consider the minimization of an objective function given access to unbiased estimates of its gradient through stochastic gradient descent (SGD) with constant step-size. While the detailed analysis was only performed for quadratic functions, we provide an explicit asymptotic expansion of the moments of the averaged SGD iterates that outlines the dependence on initial conditions, the effect of noise and the step-size, as well as the lack of convergence in the general (non-quadratic) case. For this analysis, we bring tools from Markov chain theory into the analysis of stochastic gradient and create new ones (similar but different from stochastic MCMC methods). We then show that Richardson-Romberg extrapolation may be used to get closer to the global optimum and we show empirical improvements of the new extrapolation scheme.

## 6.7. AdaBatch: Efficient Gradient Aggregation Rules for Sequential and Parallel Stochastic Gradient Methods

In [22], we study a new aggregation operator for gradients coming from a mini-batch for stochastic gradient (SG) methods that allows a significant speed-up in the case of sparse optimization problems. We call this method AdaBatch and it only requires a few lines of code change compared to regular mini-batch SGD algorithms. We provide a theoretical insight to understand how this new class of algorithms is performing and show that it is equivalent to an implicit per-coordinate rescaling of the gradients, similarly to what Adagrad methods can do. In theory and in practice, this new aggregation allows to keep the same sample efficiency of SG methods while increasing the batch size. Experimentally, we also show that in the case of smooth convex optimization, our procedure can even obtain a better loss when increasing the batch size for a fixed number of samples. We then apply this new algorithm to obtain a parallelizable stochastic gradient method that is synchronous but allows speed-up on par with Hogwild! methods as convergence does not deteriorate with the increase of the batch size. The same approach can be used to make mini-batch provably efficient for variance-reduced SG methods such as SVRG.

## 6.8. Structure-Adaptive, Variance-Reduced, and Accelerated Stochastic Optimization

In [38], we explore the fundamental structure-adaptiveness of state of the art randomized first order algorithms on regularized empirical risk minimization tasks, where the solution has intrinsic low-dimensional structure (such as sparsity and low-rank). Such structure is often enforced by non-smooth regularization or constraints. We start by establishing the fast linear convergence rate of the SAGA algorithm on non-strongly-convex objectives with convex constraints, via an argument of cone-restricted strong convexity. Then for the composite minimization task with a coordinate-wise separable convex regularization term, we propose and analyse a two stage accelerated coordinate descend algorithm (Two-Stage APCG). We provide the convergence analysis showing that the proposed method has a global convergence in general and enjoys a local accelerated linear convergence rate with respect to the low-dimensional structure of the solution. Then based on this convergence result, we proposed an adaptive variant of the two-stage APCG method which does not need to foreknow the restricted strong convexity beforehand, but estimate it on the fly. In numerical experiments we compare the adaptive two-stage APCG with various state of the art variance-reduced stochastic gradient methods on sparse regression tasks, and demonstrate the effectiveness of our approach.

## 6.9. Exponential convergence of testing error for stochastic gradient methods

In [31], we consider binary classification problems with positive definite kernels and square loss, and study the convergence rates of stochastic gradient methods. We show that while the excess testing loss (squared loss) converges slowly to zero as the number of observations (and thus iterations) goes to infinity, the testing error (classification error) converges exponentially fast if low-noise conditions are assumed.

## 6.10. Optimal algorithms for smooth and strongly convex distributed optimization in networks

In [35], we determine the optimal convergence rates for strongly convex and smooth distributed optimization in two settings: centralized and decentralized communications over a network. For centralized (i.e. *master/slave*) algorithms, we show that distributing Nesterov's accelerated gradient descent is optimal and achieves a precision  $\varepsilon > 0$  in time  $O(\sqrt{\kappa_g}(1 + \Delta \tau) \ln (1/\varepsilon))$ , where  $\kappa_g$  is the condition number of the (global) function to optimize,  $\Delta$  is the diameter of the network, and  $\tau$  (resp. 1) is the time needed to communicate values between two neighbors (resp. perform local computations). For decentralized algorithms based on gossip, we provide the first optimal algorithm, called the *multi-step dual accelerated* (MSDA) method, that achieves a precision  $\varepsilon > 0$  in time  $O(\sqrt{\kappa_l}(1 + \frac{\tau}{\sqrt{\gamma}}) \ln (1/\varepsilon))$ , where  $\kappa_l$  is the condition number of the local functions and  $\gamma$  is the (normalized) eigengap of the gossip matrix used for communication between nodes. We then verify the efficiency of MSDA against state-of-the-art methods for two problems: least-squares regression and classification by logistic regression.

## 6.11. Stochastic Composite Least-Squares Regression with convergence rate O(1/n)

In [23], we consider the minimization of composite objective functions composed of the expectation of quadratic functions and an arbitrary convex function. We study the stochastic dual averaging algorithm with a constant step-size, showing that it leads to a convergence rate of O(1/n) without strong convexity assumptions. This thus extends earlier results on least-squares regression with the Euclidean geometry to (a) all convex regularizers and constraints, and (b) all geome-tries represented by a Bregman divergence. This is achieved by a new proof technique that relates stochastic and deterministic recursions.

## 6.12. Sharpness, Restart and Acceleration

The Łojasiewicz inequality shows that sharpness bounds on the minimum of convex optimization problems hold almost generically. Sharpness directly controls the performance of restart schemes. The constants quantifying error bounds are of course unobservable, but we show in [33] that optimal restart strategies are robust, and searching for the best scheme only increases the complexity by a logarithmic factor compared to the optimal bound. Overall then, restart schemes generically accelerate accelerated methods.

## 6.13. PAC-Bayes and Domain Adaptation

In [24], we provide two main contributions in PAC-Bayesian theory for domain adaptation where the objective is to learn, from a source distribution, a well-performing majority vote on a different, but related, target distribution. Firstly, we propose an improvement of the previous approach we proposed in Germain et al. (2013), which relies on a novel distribution pseudodistance based on a disagreement averaging, allowing us to derive a new tighter domain adaptation bound for the target risk. While this bound stands in the spirit of common domain adaptation works, we derive a second bound (recently introduced in Germain et al., 2016) that brings a new perspective on domain adaptation 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. We discuss and compare both results, from which we obtain PAC-Bayesian generalization bounds. Furthermore, from the PAC-Bayesian specialization to linear classifiers, we infer two learning algorithms, and we evaluate them on real data.

## 6.14. Kernel Square-Loss Exemplar Machines for Image Retrieval

Zepeda and Pérez have recently demonstrated the promise of the exemplar SVM (ESVM) as a feature encoder for image retrieval. The paper [6] extends this approach in several directions: We first show that replacing the hinge loss by the square loss in the ESVM cost function significantly reduces encoding time with negligible effect on accuracy. We call this model square-loss exemplar machine, or SLEM. We then introduce a kernelized SLEM which can be implemented efficiently through low-rank matrix decomposition , and displays improved performance. Both SLEM variants exploit the fact that the negative examples are fixed, so most of the SLEM computational complexity is relegated to an offline process independent of the positive examples. Our experiments establish the performance and computational advantages of our approach using a large array of base features and standard image retrieval datasets.

## 6.15. Breaking the Nonsmooth Barrier: A Scalable Parallel Method for Composite Optimization

Due to their simplicity and excellent performance, parallel asynchronous variants of stochastic gradient descent have become popular methods to solve a wide range of large-scale optimization problems on multicore architectures. Yet, despite their practical success, support for nonsmooth objectives is still lacking, making them unsuitable for many problems of interest in machine learning, such as the Lasso, group Lasso or empirical risk minimization with convex constraints. In [10], we propose and analyze ProxASAGA, a fully asynchronous sparse method inspired by SAGA, a variance reduced incremental gradient algorithm. The proposed method is easy to implement and significantly outperforms the state of the art on several nonsmooth, large-scale problems. We prove that our method achieves a theoretical linear speedup with respect to the sequential version under assumptions on the sparsity of gradients and block-separability of the proximal term. Empirical benchmarks on a multi-core architecture illustrate practical speedups of up to 12x on a 20-core machine.

## 6.16. PAC-Bayesian Analysis for a two-step Hierarchical Multiview Learning Approach

In [15], we study a two-level multiview learning with more than two views under the PAC-Bayesian framework. This approach, sometimes referred as late fusion, consists in learning sequentially multiple view-specific classifiers at the first level, and then combining these view-specific classifiers at the second level. Our main theoretical result is a generalization bound on the risk of the majority vote which exhibits a term of diversity in the predictions of the view-specific classifiers. From this result it comes out that controlling the trade-off between diversity and accuracy is a key element for multiview learning, which complements other results in multiview learning.

## 6.17. Integration Methods and Accelerated Optimization Algorithms

In [37], we show that accelerated optimization methods can be seen as particular instances of multi-step integration schemes from numerical analysis, applied to the gradient flow equation. In comparison with recent advances in this vein, the differential equation considered here is the basic gradient flow and we show that multi-step schemes allow integration of this differential equation using larger step sizes, thus intuitively explaining acceleration results.

## 6.18. GANs for Biological Image Synthesis

In [17], we propose a novel application of Generative Adversarial Networks (GAN) to the synthesis of cells imaged by fluorescence microscopy. Compared to natural images, cells tend to have a simpler and more geometric global structure that facilitates image generation. However, the correlation between the spatial pattern of different fluorescent proteins reflects important biological functions, and synthesized images have to capture these relationships to be relevant for biological applications. We adapt GANs to the task at hand and propose new models with casual dependencies between image channels that can generate multi-channel images, which would be impossible to obtain experimentally. We evaluate our approach using two independent techniques and compare it against sensible baselines. Finally, we demonstrate that by interpolating across the latent space we can mimic the known changes in protein localization that occur through time during the cell cycle, allowing us to predict temporal evolution from static images.

## 6.19. Nonlinear Acceleration of Stochastic Algorithms

Extrapolation methods use the last few iterates of an optimization algorithm to produce a better estimate of the optimum. They were shown to achieve optimal convergence rates in a deterministic setting using simple gradient iterates. In [36], we study extrapolation methods in a stochastic setting, where the iterates are produced by either a simple or an accelerated stochastic gradient algorithm. We first derive convergence bounds for arbitrary, potentially biased perturbations, then produce asymptotic bounds using the ratio between the variance of the noise and the accuracy of the current point. Finally, we apply this acceleration technique to stochastic algorithms such as SGD, SAGA, SVRG and Katyusha in different settings, and show significant performance gains.

## 6.20. Algorithmic Chaining and the Role of Partial Feedback in Online Nonparametric Learning

In [20], we investigate contextual online learning with nonparametric (Lipschitz) comparison classes under different assumptions on losses and feedback information. For full information feedback and Lipschitz losses, we design the first explicit algorithm achieving the minimax regret rate (up to log factors). In a partial feedback model motivated by second-price auctions, we obtain algorithms for Lipschitz and semi-Lipschitz losses with regret bounds improving on the known bounds for standard bandit feedback. Our analysis combines novel results for contextual second-price auctions with a novel algorithmic approach based on chaining. When the context space is Euclidean, our chaining approach is efficient and delivers an even better regret bound.

## 6.21. Frank-Wolfe Algorithms for Saddle Point Problems

In [14], 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 prediction with combinatorial penalties as well as games over matching polytopes involving an exponential number of constraints.

# 6.22. Convex optimization over intersection of simple sets: improved convergence rate guarantees via an exact penalty approach

In [29], We consider the problem of minimizing a convex function over the intersection of finitely many simple sets which are easy to project onto. This is an important problem arising in various domains such as machine learning. The main difficulty lies in finding the projection of a point in the intersection of many sets. Existing approaches yield an infeasible point with an iteration-complexity of  $O(1/\varepsilon^2)$  for nonsmooth problems with no guarantees on the in-feasibility. By reformulating the problem through exact penalty functions, we derive first-order algorithms which not only guarantees that the distance to the intersection is small but also improve the complexity to  $O(1/\varepsilon)$  and  $O(1/\sqrt{\varepsilon})$  for smooth functions. For composite and smooth problems, this is achieved through a saddle-point reformulation where the proximal operators required by the primal-dual algorithms can be computed in closed form. We illustrate the benefits of our approach on a graph transduction problem and on graph matching. (Collaboration with Achintya Kundu, Francis Bach, Chiranjib Bhattacharyya)

## 6.23. A Generic Approach for Escaping Saddle points

A central challenge to using first-order methods for optimizing nonconvex problems is the presence of saddle points. First-order methods often get stuck at saddle points, greatly deteriorating their performance. Typically, to escape from saddles one has to use second-order methods. However, most works on second-order methods rely extensively on expensive Hessian-based computations, making them impractical in large-scale settings. To tackle this challenge, we introduce in [32] a generic framework that minimizes Hessian based computations while at the same time provably converging to second-order critical points. Our framework carefully alternates between a first-order and a second-order subroutine, using the latter only close to saddle points, and yields convergence results competitive to the state-of-the-art. Empirical results suggest that our strategy also enjoys a good practical performance. (Collaboration with Sashank Reddi, Manzil Zaheer, Suvrit Sra, Barnabas Poczos, Ruslan Salakhutdinov, and Alexander Smola)

# 6.24. Tracking the gradients using the Hessian: A new look at variance reducing stochastic methods

The goal of [26] is to improve variance reducing stochastic methods through better control variates. We first propose a modification of SVRG which uses the Hessian to track gradients over time, rather than to recondition, increasing the correlation of the control variates and leading to faster theoretical convergence close to the optimum. We then propose accurate and computationally efficient approximations to the Hessian, both using a diagonal and a low-rank matrix. Finally, we demonstrate the effectiveness of our method on a wide range of problems.

# 6.25. Combinatorial Penalties: Which structures are preserved by convex relaxations?

In [28] we consider the homogeneous and the non-homogeneous convex relaxations for combinatorial penalty functions defined on support sets. Our study identifies key differences in the tightness of the resulting

relaxations through the notion of the lower combinatorial envelope of a set-function along with new necessary conditions for support identification. We then propose a general adaptive estimator for convex monotone regularizers, and derive new sufficient conditions for support recovery in the asymptotic setting. (Collaboration with Marwa El Halabi, Francis Bach, Volkan Cevher)

## 6.26. On the Consistency of Ordinal Regression Methods

Many of the ordinal regression models that have been proposed in the literature can be seen as methods that minimize a convex surrogate of the zero-one, absolute, or squared loss functions. A key property that allows to study the statistical implications of such approximations is that of Fisher consistency. Fisher consistency is a desirable property for surrogate loss functions and implies that in the population setting, i.e., if the probability distribution that generates the data were available, then optimization of the surrogate would yield the best possible model. In [3] we will characterize the Fisher consistency of a rich family of surrogate loss functions used in the context of ordinal regression, including support vector ordinal regression, ORBoosting and least absolute deviation. We will see that, for a family of surrogate loss functions that subsumes support vector ordinal regression and ORBoosting, consistency can be fully characterized by the derivative of a real-valued function at zero, as happens for convex margin-based surrogates in binary classification. We also derive excess risk bounds for a surrogate of the absolute error that generalize existing risk bounds for binary classification. Finally, our analysis suggests a novel surrogate of the squared error loss. We compare this novel surrogate with competing approaches on 9 different datasets. Our method shows to be highly competitive in practice, outperforming the least squares loss on 7 out of 9 datasets.

## 6.27. Iterative hard clustering of features

In [34], we seek to group features in supervised learning problems by constraining the prediction vector coefficients to take only a small number of values. This problem includes non-convex constraints and is solved using projected gradient descent. We prove exact recovery results using restricted eigenvalue conditions. We then extend these results to combine sparsity and grouping constraints, and develop an efficient projection algorithm on the set of grouped and sparse vectors. Numerical experiments illustrate the performance of our algorithms on both synthetic and real data sets.

## 6.28. Asaga: Asynchronous Parallel Saga

In [9], 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.

### 6.29. Sparse Accelerated Exponential Weights

In [8], we consider the stochastic optimization problem where a convex function is minimized observing recursively the gradients. We introduce SAEW, a new procedure that accelerates exponential weights procedures with the slow rate  $1/\sqrt{T}$  to procedures achieving the fast rate 1/T. Under the strong convexity of the risk, we achieve the optimal rate of convergence for approximating sparse parameters in  $\mathbb{R}^d$ . The acceleration is achieved by using successive averaging steps in an online fashion. The procedure also produces sparse estimators thanks to additional hard threshold steps.

## **TAU Team**

## 7. New Results

## 7.1. Causality, Explainability, and Reliability

As said, the fairness, accountability and transparency of AI/ML need be assessed, measured and enforced to address the ethical impacts of data science on industry and society. TAU has started working toward improving the confidence in ML algorithms through three research directions.

#### 7.1.1. Causality

Links between quality of life at work and company performance Within the Amiqap project, a new approach to functional causal modeling from observational data called *Causal Generative Neural Networks* (CGNN) has been developed [45]. CGNN learns a generative model of the joint distribution of the observed variables, by minimizing the Maximum Mean Discrepancy between generated and observed data. An approximate learning criterion scales the computational cost of the approach to linear complexity in the number of observations. CGNN extensions, motivated by the redundancy of real-world variables, are under-going to achieve a causal model of the corporate- and human resource-related variables at the firm and economic sector levels.

**Generating Medical Data** This project, in collaboration with RPI (New York), aims to provide medical students with case studies, generated using CGNN . and fully preserving their confidentiality. We are exploring the benefits of using data generated by CGNNs in replacement for real data. Such data will preserve the structure of the original data, but the patient records will not represent real patients.

**Missing Data** Missing and corrupted data is a pervasive problem in data modeling. Our interest in this problem stems from 2 applications: epidemiology (in collaboration with Alain-Jacques Valleron, INSERM, and RPI New York) and computer vision (in collaboration with Aix-Marseille University and University of Barcelona). As it turns out, missing data is a causality problem [80]. In a paper under review, we outline the danger of imputing values in risk factor analysis in the presence of missing data. We are also preparing a challenge on the problem of "inpainting" to restore images with occlusions and to eliminate captions in movies.

**Power Networks** Berna Batu (post-doc Inria) explores causal modeling in time series to explain cascades of events. Other applications (e.g., in epidemiology) may develop from this approach.

#### 7.1.2. Explainability

**Explainable Machine Learning for Video Interviews** [21]. The challenge consisted in analyzing 15s videos, (human) annotated with the Big Five persinality traits (Openness to experience, Conscientiousness, Extroversion, Agreableness, and Neurotism – sometines referred to as OCEAN features). Human annotators also voted whether a given candidate should be invited for an interview. As organizers we provided a strong baseline system, which was based on deep learning methods having won part challenges. Onty the winners outperformed quantitatively the basline method.

The winner of the prediction challenge (BU-NKU) performed a very sophisticated analysis, combining face analysis (from the entire video) and scene analysis (from the first image), both analyses contributing to the final decision. Face analysis extracted spatio-temporal featured from a pre-trained convolutional neural network (CNN) and using Gabor filters. Scene analysis features were also extracted with a pre-trained CNN. Acoustic features were extracted with the OpenSMILE tool. From the feature set, the personality traits are predicted with kernel ridge regression and from there on, the "invite for interview" is predicted using Random Forests.

For the explainability challenge, the BU-NKU team performed final predictions with a classifier based on binarized predicted OCEAN scores mapped to the binarized ground truth using a decision tree, a self-explanatory model that can be converted into an explicit recommender algorithm, using the trace of each decision from the root of the tree to the leaf. The verbal explanations are finally accompanied with the aligned image from the first face-detected frame and the bar graphs of corresponding mean normalized scores. Trained on the predicted OCEAN dimensions, this gave over 90% classification accuracy.

Note that another team (TUD), who did not enter the quantitative competition, nevertheless won forst place ex-aequo with the BU-NKU team on the explainability challenge. Interestingly, they added facial features (using OpenFace) and text features (using published "Readability" features) in an effort to capture level of education from the sophistication of language, which was not captured by personality traits. They then used PCA to reduce dimension, and the coefficients of a linear regression model, fed back into the PCA model to generate explanations.

**Skin image classification** Also, the on-going collaboration with Roman Hossein Khonsari, surgeon at Necker hospital, is continuing, on the topic of skin disease image classification, with the goal of explaining how the trained neural networks produce their predictions, in order to be trusted by users. For this, we analyse the features that are learned, and show which ones are found in each image example.

### 7.1.3. Model systematic bias and reliability

A related problem is the reliability of models and their robustness to bias. We initiated research on this topic in the context of eliminating bias of Hight Energy Physics simulators. Discovering new particules relies on making accurate simulations of particle traces in detectors to diagnose collision events in high energy experiments. We are working on data from the ATLAS experiment at CERN, in collaboration with David Rousseau at the Laboratoire de l'Accelerateur Lineaire (LAL). We produced two preliminary studies on this topic: Adversarial learning to eliminate systematic errors: a case study in High Energy Physics [32] and Robust deep learning: A case study [43].

This line of research will extend to the calibration of other simulators, particularly energy transport and distribution simulators and medical data simulators, which we are working on in the context of other projects.

Beyond the calibration of simulators, we are also interested in using such approaches to forter fairness and debias data. For instance, in the "personality trait" data mentionned in the previous section, our analysis shows that labelers are biased favorably towards females (vs. males) and unfavorably towards African-American (vs. Caucasian or Asian).

## 7.2. Deep Learning and Information Theory

#### 7.2.1. Convergence proofs for recurrent networks

Pierre-Yves Massé, in his PhD, defended Dec.2017 under the supervision of Yann Ollivier [3], obtained the very first rigorous results of convergence for online training of recurrent neural networks, by viewing them from the viewpoint of dynamical systems.

#### 7.2.2. Fast algorithms for recurrent networks

Corentin Tallec (in his on-going PhD) and Yann Ollivier produced a new, faster algorithm for online training of recurrent networks, UORO, which is guaranteed to converge locally, and requires only linear time [49].

#### 7.2.3. An explanation for LSTMs

The LSTM structure is currently the most popular recurrent network architecture. However, it is quite complex and very much ad hoc. Corentin Tallec (in his on-going PhD) and Yann Ollivier derived this architecture from first principles in a very simple axiomatic setting, simply by requiring that the model is invariant to arbitrary time deformations (such as accelerations, decelerations) in the data.

#### 7.2.4. Bayesian neural networks

The Bayesian approach to neural networks makes several suggestions. First, it suggests to artificially add a very specific amount of noise during training, as a protection against overfit. This has to be done carefully (Langevin dynamics) in relation with the Fisher information metric. Gaetan Marceau-Caron and Yann Ollivier demonstrated that this approach can be applied efficiently for neural networks [28] (Best paper award at GSI17).

Second, a Bayesian viewpoint can help select the right size for each layer in a neural network. A comparison to a theoretical model of an infinitely large network suggests ways to adapt learning rates and criteria to select or deselect neurons or even layers (Preliminary results in a preprint by Pierre Wolinski (PhD), Yann Ollivier and Guillaume Charpiat, in preparation.)

### 7.2.5. Kalman filtering and information geometry

Filtering and optimization have been brought much closer by the following result [48]: the natural gradient in optimization is mathematically fully identical to the Kalman filter, for all probabilistic (machine learning) models. Even though both methods had been known for decades and were an important reference in their respective fields, they had not been brought together. The result extends to the non-iid setting (recurrent neural networks).

#### 7.2.6. Computer vision

The activity of computer vision is run jointly with the program of Looking at People (LaP) challenges [46]. We edited a book in Springer, which is a collection of tutorials and papers on gesture recognition [54], to which we contributed a survey chapter on deep-learning methods [34] a shorter version of which was published at the FG conference [17].

Several papers were published this year analyzing past LAP challenges. The "first impressions" challenge aimed at detecting personality traits from a few seconds of video. In [8], we demonstrate how deep residual networks attain state-of-the art performance on that task and lend themselves well to identifying which parts of the image is responsible for the final decision (interpretability). We also analyzed last years' challenge on apparent age estimation from in still images and proposed improvements with deep residual networks [15]. A similar methodology based on deep-residual networks was applied to apparent personality trait analysis [24], [8].

### 7.2.7. Flexible deep learning architectures suitable to genetic data

Genetic data is usually given in the form of matrices, one dimension standing for the different individuals studied and the other dimension standing for the DNA sites. These dimensions vary, depending on the indivual sample size and on the DNA sequence length. On the other side, standard deep learning architectures require data of fixed size. We consequently search for suitable, flexible architectures, with as an application the prediction of the demographic history of a population given its genetic data (changes in the number of individuals through time). Théophile Sanchez, now PhD student, presented his work at the Junior Conference on Data Science and Engineering at Paris-Saclay [33]. To our knowledge this is the first attempt in the population genetics field to learn automatically from the raw data.

#### 7.2.8. Image segmentation and classification

Emmanuel Maggiori, PhD student in the Titane team, Inria Sophia-Antipolis, mainly supervised by Yuliya Tarabalka, and co-supervised by Guillaume Charpiat, defended his PhD thesis [73], on the topic of remote sensing image segmentation with neural networks. This year, an architecture for proposed to be able to deal with high resolution images; a benchmark was built and made public (as there is lack of those in the remote sensing community); and the output of segmentation predictions was turned into a vectorial representation by suitable automatic polygonization [9], [25], [26].

Through a collaboration with the company Armadillo within the ADAMme project, we have also worked on image classification with multiple tags. The database consists of 40 millions images, with thousands of different possible tags (each image is on averaged associated with 10 tags). We started from a ResNet pretrained network and adapted it to our task. A demonstration of our results was performed at the annual review meeting of the project.

## 7.2.9. Non-rigid image alignment

Automatic image alignment was also studied. In remote sensing, the task consists in aligning satellite or aerial images with ground truth data such as OpenStreetMap's cadastrial maps. This task is crucial in that such ground truth data is actually never well registered but is spatially deformed, preventing any further use by machine learning tools. Based on the analysis of multiple scale classical frameworks, a deep learning architecture was proposed to perform this task. This work is currently under submission to CVPR. On a related topic, in a collaboration with the start-up company Therapixel, we have been studying the registration of 3D medical images, but without any ground truth or template.

#### 7.2.10. Video analysis

Time coherency is usually poorly handled in video analysis with neural networks. We have studied, on 3 different applications, different ways to take it better into account. First, in a collaboration with the Vision Institute, we studied different ways of incorporating neural networks in reinforcement learning approaches for the tracking of microbes with a motorized microscope. Second, in a collaboration with the SATIE team, we worked on the incorporation of optical flow for crowd density estimation, and, finally, in a collaboration with the Parietal team, we study how to link brain fMRI signals to the videos people are watching.

## 7.3. Algorithm Selection and Configuration

Automatic algorithm selection and configuration (hyper-parameter selection) depending on the problem instance at hand is a pervasive research topic in TAO, for both fundamental and practical reasons: in order to automatically deliver a peak performance on (nearly) every new problem instance, and to understand the specifics of a problem instance and the algorithm skills w.r.t. these specifics.

#### 7.3.1. Algorithm recommendation

A collaborative filtering approach called Alors (Algorithm Recommender System) has been proposed to achieve algorithm selection [10], considering after [81] that a problem instance "likes better" algorithms with good performances on this instance. Alors, tackling a cold-start recommendation problem, enables to independently assess the quality of the benchmark data (representativity of the problem instances w.r.t. the algorithm portfolio) and the quality of the meta-features used to describe the problem instances. Experiments on SAT, CSP and ML benchmarks yield state-of-art performances in the former two domains; these good results contrast with the poor results obtained on the ML domain, blamed on the comparatively poor quality of the ML meta-features.

#### 7.3.2. AutoML and AutoDL

Isabelle Guyon has organized the AutoML challenge (paper in preparation), proposing a series of algorithm selection and configuration problems of increasing difficulty. Following this successful challenge, a new challenge will be organized in collaboration with Google Zurich, specifically targeting the selection of deep network architectures (AutoDL: Automatic Deep learning) in five domains: Image; Video; Audio; Text; Customer demographic descriptors.

The expected result of the challenge is to alleviate the burden on data scientists to design a good architecture ("black art"), and to enforce the reproducibility of the results. In particular, this challenge will encourage advances regarding a few key research questions:

- How to make optimization algorithms more efficient without introducing more tunable parameters?
- How to efficiently automate the tuning of many hyper-parameters?
- How to automatically design or optimize a network architecture for a particular problem?
- How to further automate the learning process by directly learning how to learn?

#### 7.3.3. Per Instance Algorithm Configuration for Continuous Optimization

Nacim Belkhir's PhD thesis (defended on Nov. 30., 2017) was centered on PIAC (Per Instance Algorithm Configuration) in the context of continuous optimization. After a detailed study of features that had been proposed in the litterature, he studied the dependency of the PIAC results on the size of the sample on which they are computed. The rationale is that you must take into account the number of function evaluations that are used to compute the features when addressing a new target instance. He demonstrated that PIAC based on very small sample sets (down to 50 times the dimention) can nevertheless help improving the overall results of the optimization procedure [18], in particular by winning the single-objective track of the GECCO 2017 Black Box Competition.

### 7.3.4. Feature-based Algorithm Selection in Combinatorial Optimization

In the first part of his PhD (to be defended in Feb. 2018, see also Section 4.2), François Gonard designed ASAP, an Algorithm Selection algorithm that combines a global pre-scheduler and a per instance algorithm selector, to take advantage of the diversity of the problem instances on one hand and of the algorithms on the other hand. ASAP participated to two competitions: the 2016 ICON challenge [35], in which it obtained a *Special Mention* for its originality (and obtained excellent results on half of the problems); the 2017 OASC challenge where two versions of ASAP obtained the first overall best performances [23].

#### 7.3.5. Deep Learning calibration

In a starting collaboration with Olivier Teytaud (who left TAO for Google Zurich in 2016), we proposed [40] an online scheme for Deep Learning hyper-parameter tuning that detects and early-stops unpromising runs using extrapolation of learning curves [64], taking advantage of the parallelism, and offering optimality guarantees within the multiple hypothesis testing framework.

#### 7.3.6. Learning Rate Adaptation in Stochastic Gradient Descent

Based on an analogy with CMA-ES step-size adaptation (comparison with random walks), an original mechanism was proposed for adapting the learning rate of the stochastic gradient descent [52]. As increasing the learning rate can increase the number of catastrophic events (exploding gradients or loss values), a change detection test is used to detect such events and backtrack to safe regions. First experiments on small size problems (MNIST and CIFAR10) validate the approach. Interestingly, the same mechanism can be applied to the Adam optimizer and also improves on its basic version.

### 7.3.7. Domain Adaptation

The subject of V. Estrade's PhD is to advance domain adaptation methods in the specific context of uncertainty quantification and calibration in High Energy Physics analysis. The problem consists of learning a representation that is insensitive to perturbations induced by nuisance parameters. The need for the adversarial techniques, assuming a completely knowledge-free approach, has been questioned. Our results [32], [43] contrast the superior performance of incorporating a priori knowledge (Tangent Propagation approach) on a well separated classes problem (MNIST data) with a real case setting in HEP.

## 7.4. Generative Models and Data-driven Design

Learning generative models from observational data faces two critical issues: model selection (defining a loss criterion well suited to the considered distribution space) and tractable optimization.

### 7.4.1. A Statistical Physics Perspective

Restricted Boltzmann machines (RBM) define generative models, and advanced mean field methods of statistical physics can be leveraged to analyze the learning dynamics. Giancarlo Fissore's Master thesis (now in PhD), co-supervised by Aurélien Decelle and Cyril Furtlehner, has characterized the information content of an RBM from its spectral properties and derived a phenomenological equation of the learning process by means of the spectral dynamics of the weight matrix [5]. The learning dynamics has been analyzed in both linear and non-linear regimes, investigating the impact of the input data.

Secondly [37], the weight matrix ensemble which results from this spectral representation is used to analyze the thermodynamical properties of RBMs in terms of a phase diagram. The conditions for the RBM training, interpreted as a so-called ferromagnetic compositional phase, are given. Ferromagnetic order parameters are identified in the aforementionned phenomenological equation; a closed-form is obtained through explicit integration in simple cases, yielding a behavior of the learning spectral dynamics that matches the actual dynamics of standard RBM training (e.g. using contrastive divergence). After this model, a repulsive interaction takes place among the singular modes of the weight matrix, as some pressure of the lower modes is exerted on higher modes along training. Remarkably, this repulsive interaction is observed in algorithmic experiments for low learning rates.

### 7.4.2. Functional Brain Dynamics

Generative models have also been used by Aurélien Decelle and Cyril Furtlehner to model the dynamics of the Functional conectome (FCD) in the context of the BRAINTIME exploratory project, along two lines.

On the one hand, Restricted Boltzmann Machines have been used to learn the statistics of the time-varying resting state BOLD activity of 49 human subjects in the age span of 18 to 80 years. RBM models trained on a *per* individual basis show at least two statistically distinct pure states for each subject, between which resting state activity is stochastically wandering. Through mean-field TAP approximations of free energy we have evaluated the energy barrier between these two states *per* individual. Interestingly young and old individuals have different switching statistics: more regular for young subjects *vs* bursty and temporally irregular for elderly subjects. Furthermore, the switching probability is correlated with the energy difference between the two pure RBM states, opening the way to a personalized "landscape" analysis of the resting state FCD.

On the other hand, extremely sparse precision matrices describing the co-activation statistics of different brain regions during resting state based on BOLD time-series have been derived using sparse Gaussian copula models. Such extremely sparse models support direct inter-subject comparisons, in contrast with usually dense FC descriptions. A further step is to characterize the brain activity dynamics, e.g. through considering multi-temporal slice models.

#### 7.4.3. Power systems Design and Optimization

Last work within the POST project, Vincent Berthier's PhD [2] addressed issues in global continuous optimization, and proposed to use unit commitment problems to go beyond classical benchmarks of analytical functions.

Benjamin Donnot (RTE Cifre PhD, now under Isabelle Guyon's supervision), successfully started to disseminate his work in the power system community [20]. His main results regard the design of an original alternative to the one-hot encoding for the topology of the French power grid, termed *Guided Dropout*. Taking advantate of the high redundancy of network connections, the idea is to learn a random mapping between all possible "n-1" topologies and the connections of the neurons [65], [42].

#### 7.4.4. Multi-Objective Optimization

**Dynamic Objectives**: Within the E-Lucid project, coordinated by Thales Communications & Security, the on-going work about anomaly detection in network flow [74] led to an original approach to many-objective problem, where the objectives are gradually introduced, preventing the population to be abruptly driven toward satisficing only the easy objectives at the beginning of the evolution [27] (runner-up for the Best Paper Award of the Evolutionary Multi-Objective track at GECCO 2017).

**Dynamic Fitness Cases:** In [22], we propose to gradually introduce the fitness cases in the case of symbolic regression with Genetic Programming, so as to guide the search more smoothly. Experimental results demonstrate a better success rate in the case of both static and dynamic problems.

## 7.4.5. Space Weather Forecasting

In the context of the MDG-TAU joint team project, focusing on space weather forecasting, Mhamed Hajaiej's Master thesis (under Aurélien Decelle, Cyril Furtlehner and Michèle Sebag's supervision) has tackled the prediction of magnetic storms from solar magnetograms, more specifically considering the representation of solar magnetograms based on auto-encoders. Besides finding a well-suited NN architecture, the difficulty was to find a loss function well suited to the data distribution. A next step (Mandar Chandorkar's PhD at CWI under Enrico Camporeale supervision) is to estimate from the solar images the speed of the solar wind, and the time needed for solar storms to reach the first Lagrange point; this estimation is meant to build a well-defined supervised learning problem, associating a solar image at t to its effect measured at  $t + \delta$  on the first Lagrange point.

## **ASPI Team**

## 5. New Results

## 5.1. Central limit theorem for adaptive multilevel splitting

Participants: Frédéric Cérou, Arnaud Guyader, Mathias Rousset.

See 3.2, and 4.2.

This is a collaboration with Bernard Delyon (université de Rennes 1).

Fleming–Viot type particle systems represent a classical way to approximate the distribution of a Markov process with killing, given that it is still alive at a final deterministic time. In this context, each particle evolves independently according to the law of the underlying Markov process until its killing, and then branches instantaneously on another randomly chosen particle. While the consistency of this algorithm in the large population limit has been recently studied in several articles, our purpose here is to prove central limit theorems under very general assumptions. For this, we only suppose that the particle system does not explode in finite time, and that the jump and killing times have atomless distributions. In particular, this includes the case of elliptic diffusions with hard killing.

## 5.2. Adaptive multilevel splitting for Monte Carlo particle transport

Participant: Mathias Rousset.

#### See 3.2, and 4.2.

Simulation of neutron transport with Monte Carlo methods is a central issue in order to assess the aging of french nucelar plants.

In [49], we propose an alternative version of the AMS (adaptive multilevel splitting) algorithm, adapted for the first time to the field of particle tranport. Within this context, it can be used to build an unbiased estimator of any quantity associated with particle tracks, such as flux, reaction rates or even non–Boltzmann tallies. Furthermore, the effciency of the AMS algorithm is shown not to be very sensitive to variations of its input parameters, which makes it capable of significant variance reduction without requiring extended user effort.

## 5.3. Weak overdamped limit theorem for Langevin processes

Participant: Mathias Rousset.

This is a collaboration with Pierre-André Zitt (université Paris Est Marne-la-Vallée).

The Langevin stochastic process is the main model used in molecular dynamics simulation, for instance for the simulation of reactive trajectories of bio-chemical systems with rare event techniques.

In [21], we prove convergence in distribution of Langevin processes in the overdamped diffusion asymptotics. The proof relies on the classical perturbed test function (or corrector) method, which is used both to show tightness in path space, and to identify the extracted limit with a martingale problem. The result holds assuming the continuity of the gradient of the potential energy, and a mild control of the initial kinetic energy.

## 5.4. Particle–Kalman filter for structural health monitoring

Participant: Frédéric Cérou.

This is a joint work with EPI I4S (Inria Rennes-Bretagne Atlantique).

Standard filtering techniques for structural parameter estimation assume that the input force either is known exactly or can be replicated using a known white Gaussian model. Unfortunately for structures subjected to seismic excitation, the input time history is unknown and also no previously known representative model is available. This invalidates the aforementioned idealization. To identify seismic induced damage in such structures using filtering techniques, a novel algorithm is proposed to estimate the force as additional state in parallel to the system parameters. Two concurrent filters are employed for parameters and force respectively. For the parameters, interacting particle–Kalman filter is employed targeting systems with correlated noise. Alongside a second filter is employed to estimate the seismic force acting on the structure. The proposal is numerically validated on a sixteen degrees–of–freedom mass–spring–damper system. The estimation results confirm the applicability of the proposed algorithm.

In another work, the same approach has been used for varying system parameters with correlated state and observation noise. The idea is to nest a bank of linear KFs (Kalman filters) for state estimation within a PF (particle filter) environment that estimates the parameters. This facilitates employing relatively less expensive linear KF for linear state estimation problem while costly PF is employed only for parameter estimation. Additionally, the proposed algorithm also takes care of those systems for which system and measurement noises are not uncorrelated as it is commonly idealized in standard filtering algorithms. As an example, for mechanical systems under ambient vibration it happens when acceleration response is considered as measurement. Thus the process and measurement noise in these system descriptions are obviously correlated. For this, an improved description for the Kalman gain is developed. Further, to enhance the consistency of particle filtering based parameter estimation involving high dimensional parameter space, a new temporal evolution strategy for the particles is defined. This strategy aims at restricting the solution from diverging (up to the point of no return) because of an isolated event of infeasible estimation which is very much likely especially when dealing with high dimensional parameter space.

### 5.5. Reduced modeling of unknown trajectories

Participant: Patrick Héas.

This is a collaboration with Cédric Herzet (EPI FLUMINANCE, Inria Rennes-Bretagne Atlantique)

In [12], we deal with model order reduction of parametrical dynamical systems. We consider the specific setup where the distribution of the system's trajectories is unknown but the following two sources of information are available: (*i*) some "rough" prior knowledge on the system's realisations, and (*ii*) a set of "incomplete" observations of the system's trajectories. We propose a Bayesian methodological framework to build reduced–order models (ROMs) by exploiting these two sources of information.

We emphasise that complementing the prior knowledge with the collected data provably enhances the knowledge of the distribution of the system's trajectories. We then propose an implementation of the proposed methodology based on Monte Carlo methods. In this context, we show that standard ROM learning techniques, such as proper orthogonal decomposition (POD) or dynamic mode decomposition (DMD), can be revisited and recast within the probabilistic framework considered in this work. We illustrate the performance of the proposed approach by numerical results obtained for a standard geophysical model.

## 5.6. Model reduction from partial observations

Participant: Patrick Héas.

This is a collaboration with Angélique Drémeau (ENSTA Bretagne, Brest) and Cédric Herzet (EPI FLUMI-NANCE, Inria Rennes–Bretagne Atlantique)

In [11], we deal with model-order reduction of parametric partial differential equations (PPDE). More specifically, we consider the problem of finding a good approximation subspace of the solution manifold of the PPDE when only partial information on the latter is available. We assume that two sources of information are available: i) a "rough" prior knowledge, taking the form of a manifold containing the target solution manifold, and ii) partial linear measurements of the solutions of the PPDE (the term partial refers

to the fact that observation operator cannot be inverted). We provide and study several tools to derive good approximation subspaces from these two sources of information. We first identify the best worst-case performance achievable in this setup and propose simple procedures to approximate the corresponding optimal approximation subspace. 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.

## 5.7. Low–rank dynamic mode decomposition: optimal solution in polynomial time

Participant: Patrick Héas.

This is a collaboration with Cédric Herzet (EPI FLUMINANCE, Inria Rennes-Bretagne Atlantique)

The works [15] and [41] study the linear approximation of high–dimensional dynamical systems using low-rank dynamic mode decomposition (DMD). Searching this approximation in a data–driven approach can be formalised as attempting to solve a low-rank constrained optimisation problem. This problem is non–convex and state–of–the–art algorithms are all sub–optimal. We show that there exists a closed-form solution, which can be computed in polynomial time, and characterises the  $\ell_2$ –norm of the optimal approximation error. The theoretical results serve to design low–complexity algorithms building reduced models from the optimal solution, based on singular value decomposition or low–rank DMD. The algorithms are evaluated by numerical simulations using synthetic and physical data benchmarks.

## 5.8. Optimal kernel-based dynamic mode decomposition

Participant: Patrick Héas.

This is a collaboration with Cédric Herzet (EPI FLUMINANCE, Inria Rennes-Bretagne Atlantique)

The state–of–the–art algorithm known as kernel-based dynamic mode decomposition (K–DMD) provides a sub–optimal solution to the problem of reduced modeling of a dynamical system based on a finite approximation of the Koopman operator. It relies on crude approximations and on restrictive assumptions. The purpose of the work in [20] is to propose a kernel–based algorithm solving exactly this low–rank approximation problem in a general setting.

### 5.9. Non parametric state–space model for missing–data imputation

Participants: Thi Tuyet Trang Chau, François Le Gland, Valérie Monbet, Mathias Rousset.

This is a collaboration with Pierre Ailliot (université de Bretagne Occidentale, Brest), Ronan Fablet and Pierre Tandéo (Télécom Bretagne, Brest), Anne Cuzol (université de Bretagne Sud, Vannes) and Bernard Chapron (IFREMER, Brest).

Missing data are present in many environmental data–sets and this work aims at developing a general method for imputing them. State–space models (SSM) have already extensively been used in this framework. The basic idea consists in introducing the true environmental process, which we aim at reconstructing, as a latent process and model the data available at neighboring sites in space and/or time conditionally to this latent process. A key input of SSMs is a stochastic model which describes the temporal evolution of the environmental process of interest. In many applications, the dynamic is complex and can hardly be described using a tractable parametric model. Here we investigate a data-driven method where the dynamical model is learned using a non-parametric approach and historical observations of the environmental process of interest. From a statistical point of view, we will address various aspects related to SSMs in a non–parametric framework. First we will discuss the estimation of the filtering and smoothing distributions, that is the distribution of the latent space given the observations, using sequential Monte Carlo approaches in conjunction with local linear regression. Then, a more difficult and original question consists in building a non–parametric estimate of the dynamics which takes into account the measurement errors which are present in historical data. We will propose an EM–like algorithm where the historical data are corrected recursively. The methodology will be illustrated and validated on an univariate toy example.

## **CQFD Project-Team**

## 7. New Results

## 7.1. Asymptotically optimal open-loop load balancing

In many distributed computing systems, stochastically arriving jobs need to be assigned to servers with the objective of minimizing waiting times. Many existing dispatching algorithms are basically included in the SQ(d) framework: Upon arrival of a job,  $d \ge 2$  servers are contacted uniformly at random to retrieve their state and then the job is routed to a server in the best observed state. One practical issue in this type of algorithm is that server states may not be observable, depending on the underlying architecture. In [3], we investigate the assignment problem in the open-loop setting where no feedback information can flow dynamically from the queues back to the controller, i.e., the queues are unobservable. This is an intractable problem, and unless particular cases are considered, the structure of an optimal policy is not known. Under mild assumptions and in a heavy-traffic many-server limiting regime, our main result proves the optimality of a subset of deterministic and periodic policies within a wide set of (open-loop) policies that can be randomized or deterministic and can be dependent on the arrival process at the controller. The limiting value of the scaled stationary mean waiting time achieved by any policy in our subset provides a simple approximation for the optimal system performance.

Author: J. Anselmi (Inria CQFD).

## 7.2. The economics of the cloud: price competition and congestion

The work developed in [4] proposes a model to study the interaction of price competition and congestion in the cloud computing marketplace. Specifically, we propose a three-tier market model that captures a marketplace with users purchasing services from Software-as-Service (SaaS) providers, which in turn purchase computing resources from either Provider-as-a-Service (PaaS) providers or Infrastructure-as-a-Service (IaaS) providers. Within each level, we define and characterize competitive equilibria. Further, we use these characterizations to understand the relative profitability of SaaSs and PaaSs/IaaSs, and to understand the impact of price competition on the user experienced performance, i.e., the 'price of anarchy' of the cloud marketplace. Our results highlight that both of these depend fundamentally on the degree to which congestion results from shared or dedicated resources in the cloud.

Authors: J. Anselmi (Inria CQFD), D. Ardagna, J.C.S. Lui, A. Wierman, Y. Xu and Z. Yang.

## 7.3. A new characterization of the jump rate for piecewise-deterministic Markov processes with discrete transitions

Piecewise-deterministic Markov processes form a general class of non-diffusion stochastic models that involve both deterministic trajectories and random jumps at random times. In [5], we state a new characterization of the jump rate of such a process with discrete transitions. We deduce from this result a nonparametric technique for estimating this feature of interest. We state the uniform convergence in probability of the estimator. The methodology is illustrated on a numerical example.

Authors: A. Genadot (Inria CQFD) and R. Azais.

## 7.4. Linear minimum mean square filters for Markov jump linear systems

In [9], new linear minimum mean square estimators are introduced by considering a cluster information structure in the filter design. The set of filters constructed in this way can be ordered in a lattice according to the refines of clusters of the Markov chain, including the linear Markovian estimator at one end (with only one cluster) and the Kalman filter at the other hand (with as many clusters as Markov states). The higher is the number of clusters, the heavier are pre-computations and smaller is the estimation error, so that the cluster cardinality allows for a trade-off between performance and computational burden. In this paper we propose the estimator, give the formulas for pre-computation of gains, present some properties, and give an illustrative numerical example.

Authors: E. Costa and B. De Saporta (Inria CQFD).

## 7.5. Zero-sum discounted reward criterion games for piecewise deterministic Markov processes

In [10], we deal with zero-sum games with a discounted reward criterion for piecewise deterministic Markov process (PDMPs) in general Borel spaces. The two players can act on the jump rate and transition measure of the process, with the decisions being taken just after a jump of the process. The goal of this paper is to derive conditions for the existence of minâmax strategies for the infinite horizon total expected discounted reward function, which is composed of running and boundary parts. The basic idea is, by using the special features of the PDMPs, to re-write the problem via an embedded discrete-time Markov chain associated to the PDMP and re-formulate the problem as a discrete-stage zero sum game problem.

Authors: O. Costa and F. Dufour (Inria CQFD).

# 7.6. Optimal strategies for impulse control of piecewise deterministic Markov processes

In [11], we deal with the general discounted impulse control problem of a piecewise deterministic Markov process. We investigate a new family of optimal strategies. The construction of such strategies is explicit and only necessitates the previous knowledge of the cost of the no-impulse strategy. In particular, it does not require the resolution of auxiliary optimal stopping problem or the computation of the value function at each point of the state space. This approach is based on the iteration of a single-jump-orintervention operator associated to the piecewise deterministic Markov process.

Authors: B. De Saporta, F. Dufour and A. Geeraert. All authors are members of CQFD at Inria.

# 7.7. Partially observed optimal stopping problem for discrete-time Markov processes

In [12], we have investigated of a new numerical method to approximate the optimal stopping problem for a discrete-time continuous state space Markov chain under partial observations. It is based on a two-step discretization procedure based on optimal quantization. First, we discretize the state space of the unobserved variable by quantizing an underlying reference measure. Then we jointly discretize the resulting approximate filter and the observation process. We obtain a fully computable approximation of the value function with explicit error bounds for its convergence towards the true value fonction.

Authors: B. De Saporta, F. Dufour and C. Nivot. All authors are members of CQFD at Inria.

# 7.8. On the stability and the uniform propagation of chaos of a class of extended ensemble Kalman–Bucy filters

The result published in [15] deals with the exponential stability and the uniform propagation of chaos properties of a class of Extended Ensemble Kalman-Bucy filters with respect to the time horizon. This class of nonlinear filters can be interpreted as the conditional expectations of nonlinear McKean Vlasov type diffusions with respect to the observation process. In contrast with more conventional Langevin nonlinear drift type processes, the mean field interaction is encapsulated in the covariance matrix of the diffusion. The main results discussed in the article are quantitative estimates of the exponential stability properties of these nonlinear diffusions. These stability properties are used to derive uniform and non asymptotic estimates of the propagation of chaos properties of Extended Ensemble Kalman filters, including exponential concentration inequalities. To our knowledge these results seem to be the first results of this type for this class of nonlinear ensemble type Kalman-Bucy filters.

Authors: P. Del Moral (Inria CQFD), A. Kurtzmann and J. Tugaut.

# 7.9. Exponential mixing properties for time inhomogeneous diffusion processes with killing

In [16], we consider an elliptic and time-inhomogeneous diffusion process with time-periodic coefficients evolving in a bounded domain of R d 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 evolution operator; 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.

Authors: P. Del Moral (Inria CQFD) and D. Villemonais.

### 7.10. Averaging for some simple constrained Markov processes

In [17], we study a class of piecewise deterministic Markov processes with underlying fast dynamic. Using a " penalty method ", an averaging result is obtained when the underlying dynamic is infinitely accelerated. The features of the averaged process, which is still a piecewise deterministic Markov process, are fully described.

Authors: A. Genadot (Inria CQFD).

## 7.11. Nonasymptotic analysis of adaptive and annealed Feynman–Kac particle models

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 [18], 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.

Authors: F. Giraud and P. Del Moral (Inria CQFD).

## 7.12. A comparison of fitness-case sampling methods for genetic programming

Genetic programming (GP) is an evolutionary computation paradigm for automatic program induction. GP has produced impressive results but it still needs to overcome some practical limitations, particularly its high computational cost, overfitting and excessive code growth. Recently, many researchers have proposed fitness-case sampling methods to overcome some of these problems, with mixed results in several limited tests. In [20], we present an extensive comparative study of four fitness-case sampling methods, namely: Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and Keep-Worst Interleaved Sampling. The algorithms are compared on 11 symbolic regression problems and 11 supervised classification problems, using 10 synthetic benchmarks and 12 real-world data-sets. They are evaluated based on test performance, overfitting and average program size, comparing them with a standard GP search. Comparisons are carried out using non-parametric multigroup tests and post hoc pairwise statistical tests. The experimental results suggest that fitness-case sampling methods are particularly useful for difficult real-world symbolic regression problems, improving performance, reducing overfitting and limiting code growth. On the other hand, it seems that fitness-case sampling cannot improve upon GP performance when considering supervised binary classification.

Authors: Y. Martinez, E. Naredo, L. Trujillo, P. Legrand (Inria CQFD) and U. Lopez.

# 7.13. Stochastic control of observer trajectories in passive tracking with acoustic signal propagation optimization

In [23], we present a numerical method which computes the optimal trajectory of a underwater vehicle subject to some mission objectives. The method is applied to a submarine whose goal is to best detect one or several targets, or/and to minimize its own detection range perceived by the other targets. The signal considered is acoustic propagation attenuation. Our approach is based on dynamic programming of a finite horizon Markov decision process. A quantization method is applied to fully discretize the problem and allows a numerically tractable solution. Different scenarios are considered. We suppose at first that the position and the velocity of the targets are known and in the second we suppose that they are unknown and estimated by a Kalman type filter in a context of bearings-only tracking.

Authors: H. Zhang (Inria CQFD), B. De Saporta (Inria CQFD), F. Dufour (Inria CQFD), D. Laneuville and A. Nègre.

## 7.14. Use of local Search in Genetic Programming

There are two important limitations of standard tree-based genetic programming (GP). First, GP tends to evolve unnecessarily large programs, what is referred to as bloat. Second, GP uses inefficient search operators that focus on modifying program syntax. The first problem has been studied in many works, with many bloat control proposals. Regarding the second problem, one approach is to use alternative search operators, for instance geometric semantic operators, to improve convergence. In [36], our goal is to experimentally show that both problems can be effectively addressed by incorporating a local search optimizer as an additional search operator. Using real-world problems, we show that this rather simple strategy can improve the convergence and performance of tree-based GP, while reducing program size. Given these results, a question arises: why are local search strategies so uncommon in GP? A small survey of popular GP libraries suggests to us that local search is underused in GP systems.

Authors: Leonardo Trujillo, Emigdio Z-Flores, Perla S. Juarez Smith, Pierrick Legrand (Inria CQFD), Sara Silva, Mauro Castelli, Leonardo Vanneschi, Oliver Schutze and Luis Munoz.

## 7.15. Hierarchical clustering with spatial constraints

In [8], we propose a Ward-like hierarchical clustering algorithm including spatial/geographical constraints. Two dissimilarity matrices  $D_0$  and  $D_1$  are inputted, along with a mixing parameter  $\alpha \in [0, 1]$ . The dissimilarities can be non-Euclidean and the weights of the observations can be non-uniform. The first matrix gives the dissimilarities in the "feature space" and the second matrix gives the dissimilarities in the "constraint space". The criterion minimized at each stage is a convex combination of the homogeneity criterion calculated with  $D_0$  and the homogeneity criterion calculated with  $D_1$ . The idea is then to determine a value of  $\alpha$  which increases the spatial contiguity without deteriorating too much the quality of the solution based on the variables of interest i.e. those of the feature space. This procedure is illustrated on a real dataset using the R package ClustGeo.

Authors: Marie Chavent (Inria CQFD), Vanessa Kuentz, Amaury Labenne, Jérôme Saracco (Inria CQFD).

# 7.16. Variable importance assessment in sliced inverse regression for variable selection

In [19], we are interested in treating the relationship between a dependent variable y and a multivariate covariate x in a semiparametric regression model. Since the purpose of most social, biological, or environmental science research is the explanation, the determination of the importance of the variables is a major concern. It is a way to determine which variables are the most important when predicting y. Sliced inverse regression methods allows to reduce the space of the covariate x by estimating the directions  $\beta$  that form an effective dimension reduction (EDR) space. The aim of this article is to propose a computational method based on importance variable measure (only relying on the EDR space) in order to select the most useful variables. The numerical behavior of this new method, implemented in R, is studied on a simulation study. An illustration on a real data is also provided.

Authors: Ines Jlassi, Jérôme Saracco (Inria CQFD).

## 7.17. Group-sparse block PCA and explained variance

In [46], we address the simultaneous determination of group-sparse loadings by block optimization, and the correlated problem of defining explained variance for a set of non orthogonal components. We give in both cases a comprehensive mathematical presentation of the problem, which leads to propose i) a new formulation/algorithm for group-sparse block PCA and ii) a framework for the definition of explained variance with the analysis of five definitions. The numerical results i) confirm the superiority of block optimization over deflation for the determination of group-sparse loadings, and the importance of group information when available, and ii) show that ranking of algorithms according to explained variance is essentially independent of the definition of explained variance. These results lead to propose a new optimal variance as the definition of choice for explained variance.

Authors: Guy Chavent, Marie Chavent (Inria CQFD).

## 7.18. Multivariate Analysis of Mixed Data

In [47], we focus on mixed data that arise when observations are described by a mixture of numerical and categorical variables. The R package PCAmixdata extends standard multivariate analysis methods to incorporate this type of data. The key techniques/methods included in the package are principal component analysis for mixed data (PCAmix), varimax-like orthogonal rotation for PCAmix, and multiple factor analysis for mixed multi-table data. This paper gives a synthetic presentation of the three algorithms with details to help the user understand graphical and numerical outputs of the corresponding R functions. The three main methods are illustrated on a real dataset composed of four data tables characterizing living conditions in different municipalities in the Gironde region of southwest France.

Authors: Marie Chavent (Inria CQFD), Vanessa Kuentz, Amaury Labenne, Jérôme Saracco (Inria CQFD).

## 7.19. A Smooth Nonparametric Estimator of a Conditional Quantile

In [50], we propose a new smooth nonparametric estimator of conditional quantile of Y for a given value of X using a kernel type of estimators. A numerical study to examine the performance of our estimator as well as a theoretical asymptotic study have been conducted.

Authors: Ines Jlassi, Jérôme Saracco (Inria CQFD).

## 7.20. Perturbations and projections of Kalman-Bucy semigroups

The purpose of the work published in [40] is to analyse the effect of various perturbations and projections of Kalman-Bucy semigroups and Riccati equations. The original motivation was to understand the behaviour of various regulation methods used in ensemble Kalman filtering (EnKF). For example, covariance inflation-type methods (perturbations) and covariance localisation methods (projections) are commonly used in the EnKF literature to ensure well-posedness of the sample covariance (e.g. sufficient rank) and to 'move' the sample covariance closer (in some sense) to the Riccati flow of the true Kalman filter. In the limit, as the number of samples tends to infinity, these methods drive the sample covariance toward a solution of a perturbed, or projected, version of the standard (Kalman-Bucy) differential Riccati equation. The behaviour of this modified Riccati equation is investigated here. Results concerning continuity (in terms of the perturbations), boundedness, and convergence of the Riccati flow to a limit are given. In terms of the limiting filters, results characterising the error between the perturbed/projected and nominal conditional distributions are given. New projection-type models and ideas are also discussed within the EnKF framework; e.g. projections onto socalled Bose-Mesner algebras. This work is generally important in understanding the limiting bias in both the EnKF empirical mean and covariance when applying regularisation. Finally, we note the perturbation and projection models considered herein are also of interest on their own, and in other applications such as differential games, control of stochastic and jump processes, and robust control theory, etc.

Authors: Pierre Del Moral (Inria CQFD), Adrian Bishop and Sahani Pathiraja.

# 7.21. Probabilistic Safety Analysis of the Collision Between a Space Debris and a Satellite with an Island Particle Algorithm

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 o 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 inuence of dierent simulation parameters (such as the drag coecient) that are set for to simplify the simulation, on the collision 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.

Authors: Pierre Del Moral (Inria CQFD), Christelle Vergé, Jérôme Morio and Juan Carlos Dolado Pérez.

### 7.22. Biased online parameter inference for state-space models

We consider Bayesian online static parameter estimation for state-space models. This is a very important problem, but is very computationally challenging as the state-of-the art methods that are exact, often have a computational cost that grows with the time parameter; perhaps the most successful algorithm is that of SM C2 (Chopin et al., J R Stat Soc B 75: 397–426 2013). We present a version of the SM C2 algorithm

which has computational cost that does not grow with the time parameter. In addition, under assumptions, the algorithm is shown to provide consistent estimates of expectations w.r.t. the posterior. However, the cost to achieve this consistency can be exponential in the dimension of the parameter space; if this exponential cost is avoided, typically the algorithm is biased. The bias is investigated from a theoretical perspective and, under assumptions, we find that the bias does not accumulate as the time parameter grows. The algorithm is implemented on several Bayesian statistical models.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Yan Zhou.

## 7.23. Multilevel Sequential Monte Carlo Samplers for Normalizing Constants

This work considers the sequential Monte Carlo (SMC) approximation of ratios of normalizing constants associated to posterior distributions which in principle rely on continuum models. Therefore, the Monte Carlo estimation error and the discrete approximation error must be balanced. A multilevel strategy is utilized to substantially reduce the cost to obtain a given error level in the approximation as compared to standard estimators. Two estimators are considered and relative variance bounds are given. The theoretical results are numerically illustrated for the example of identifying a parametrized permeability in an elliptic equation given point-wise observations of the pressure.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra, Kody Law and Yan Zhou.

# 7.24. Multilevel sequential Monte Carlo: Mean square error bounds under verifiable conditions

In this article, we consider the multilevel sequential Monte Carlo (MLSMC) method of Beskos et al. (Stoch. Proc. Appl. [to appear]). This is a technique designed to approximate expectations w.r.t. probability laws associated to a discretization. For instance, in the context of inverse problems, where one discretizes the solution of a partial differential equation. The MLSMC approach is especially useful when independent, coupled sampling is not possible. Beskos et al. show that for MLSMC the computational effort to achieve a given error, can be less than independent sampling. In this article we significantly weaken the assumptions of Beskos et al., extending the proofs to non-compact state-spaces. The assumptions are based upon multiplicative drift conditions as in Kontoyiannis and Meyn (Electron. J. Probab. 10 [2005]: 61–123). The assumptions are verified for an example.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Kody Law.

## 7.25. Biased Online Parameter Inference for State-Space Models

We consider Bayesian online static parameter estimation for state-space models. This is a very important problem, but is very computationally challenging as the state-of-the art methods that are exact, often have a computational cost that grows with the time parameter; perhaps the most successful algorithm is that of SM C2 (Chopin et al., J R Stat Soc B 75: 397–426 2013). We present a version of the SM C2 algorithm which has computational cost that does not grow with the time parameter. In addition, under assumptions, the algorithm is shown to provide consistent estimates of expectations w.r.t. the posterior. However, the cost to achieve this consistency can be exponential in the dimension of the parameter space; if this exponential cost is avoided, typically the algorithm is biased. The bias is investigated from a theoretical perspective and, under assumptions, we find that the bias does not accumulate as the time parameter grows. The algorithm is implemented on several Bayesian statistical models.

Authors: Pierre Del Moral (Inria CQFD), Ajay Jasra and Yan Zhou.

# 7.26. Valuation of Barrier Options using Sequential Monte Carlo

Sequential Monte Carlo (SMC) methods have successfully been used in many applications in engineering, statistics and physics. However, these are seldom used in financial option pricing literature and practice. This paper presents SMC method for pricing barrier options with continuous and discrete monitoring of the barrier condition. Under the SMC method, simulated asset values rejected due to barrier condition are re-sampled from asset samples that do not breach the barrier condition improving the efficiency of the option price estimator; while under the standard Monte Carlo many simulated asset paths can be rejected by the barrier condition making it harder to estimate option price accurately. We compare SMC with the standard Monte Carlo method and demonstrate that the extra effort to implement SMC when compared with the standard Monte Carlo is very little while improvement in price estimate can be significant. Both methods result in unbiased estimators for the price converging to the true value as  $1/\sqrt{M}$ , where M is the number of simulations (asset paths). However, the variance of SMC estimator is smaller and does not grow with the number of time steps when compared to the standard Monte Carlo. In this paper we demonstrate that SMC can successfully be used for pricing barrier options. SMC can also be used for pricing other exotic options and also for cases with many underlying assets and additional stochastic factors such as stochastic volatility; we provide general formulas and references.

Authors: Pierre Del Moral (Inria CQFD) and Pavel V. Shevchenko.

# **MATHRISK Project-Team**

# 6. New Results

### 6.1. Systemic risk

Participants: Agnès Sulem, Andreea Minca [Cornell University], Rui Chen.

We have studied optimal connectivity of a large financial network in presence of growth and contagion [27]. We obtained asymptotic results for the magnitude of default contagion in a large financial system with intrinsic recovery features in the framework of a random network. We have moreover added a game component to the model, allowing institutions to choose their optimal linkages in order to maximize their final profits, given their initial states and estimated survival probabilities.

# 6.2. Optimal stopping for Backward stochastic (partial) differential equations with jumps

Agnès Sulem, Rui Chen and R. Dumitrescu have addressed the problem of optimal stopping for general meanfield backward stochastic differential equations driven by a Brownian motion and an independent Poisson random measure. Existence, uniqueness, comparison and dual representation results have been obtained. Links with reflected mean-field BSDEs have been established and application to global dynamic risk measure theory has been investigated.

American options in markets with imperfections and default have been studied by Agnès Sulem, M.C. Quenez and R. Dumitrescu [28].

## 6.3. Approximation of Martingale Optimal Transport problems

With J. Corbetta, A. Alfonsi and B. Jourdain study sampling methods preserving the convex order for two probability measures  $\mu$  and  $\nu$  on  $\mathbb{R}^d$ , with  $\nu$  dominating  $\mu$ . When  $(X_i)_{1 \le i \le I}$  (resp.  $(Y_j)_{1 \le j \le J}$ ) are independent dent and identically distributed according  $\mu$  (resp.  $\nu$ ), in general  $\mu_I = \frac{1}{I} \sum_{i=1}^{-T} \delta_{X_i}$  and  $\nu_J = \frac{1}{J} \sum_{j=1}^{J} \delta_{Y_j}$  are not rankable for the convex order. They investigate modifications of  $\mu_I$  (resp.  $\nu_J$ ) smaller than  $\nu_J$  (resp. greater than  $\mu_I$  in the convex order and weakly converging to  $\mu$  (resp.  $\nu$ ) as  $I, J \to \infty$ . They first consider the one dimensional case d = 1, where, according to Kertz and Rösler, the set of probability measures with a finite first order moment is a lattice for the increasing and the decreasing convex orders. Given  $\mu$  and  $\nu$  in this set, they define  $\mu \lor \nu$  (resp.  $\mu \land \nu$ ) as the supremum (resp. infimum) of  $\mu$  and  $\nu$  for the decreasing convex order when  $\int_{\mathbf{R}} x\mu(dx) \leq \int_{\mathbf{R}} x\nu(dx)$  and for the increasing convex order otherwise. This way,  $\mu \vee \nu$  (resp.  $\mu \wedge \nu$ ) is greater than  $\mu$  (resp. smaller than  $\nu$ ) in the convex order. They give efficient algorithms permitting to compute  $\mu \lor \nu$  and  $\mu \land \nu$  (and therefore  $\mu_I \lor \nu_J$  and  $\mu_I \land \nu_J$ ) when  $\mu$  and  $\nu$  are convex combinations of Dirac masses. In general dimension, when  $\mu$  and  $\nu$  have finite moments of order  $\rho \ge 1$ , they define the projection  $\mu \downarrow_{\rho} \nu$ (resp.  $\mu \uparrow_{\rho} \nu$ ) of  $\mu$  (resp.  $\nu$ ) on the set of probability measures dominated by  $\nu$  (resp. larger than  $\mu$ ) in the convex order for the Wasserstein distance with index  $\rho$ . When  $\rho = 2$ ,  $\mu_I \downarrow_2 \nu_J$  can be computed efficiently by solving a quadratic optimization problem with linear constraints. It turns out that, in dimension d = 1, the projections do not depend on  $\rho$  and their quantile functions are explicit in terms of those of  $\mu$  and  $\nu$ , which leads to efficient algorithms for convex combinations of Dirac masses. Last, they illustrate by numerical experiments the resulting sampling methods that preserve the convex order and their application to approximate Martingale Optimal Transport problems.

With V. Ehrlacher, D. Lombardi and R. Coyaud, A. Alfonsi has started to develop and analyze numerical methods to approximate the optimal transport between two probability measures.

## 6.4. Numerical methods for Asset-Liability Management

With A. Cherchali, A. Alfonsi is working on obtaining a model for the Asset-Liability Management (ALM) of insurance companies. The purpose is to use this model to develop Monte-Carlo methods to approximate the SCR (Solvency Capital Requirement).

## 6.5. American options

With Giulia Terenzi, D. Lamberton has been working on American options in Heston's model. Some 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) have been obtained, as well as some results on monotonicity and regularity properties of the price function. A paper on this topic has just been submitted.

## 6.6. Stochastic Analysis and Malliavin calculus

• Invariance principles for stochastic polynomials [40].

With L. Caramellino (Roma), V. Bally has studied invariance principles for stochastic polynomials. This is a generalization of the classical invariance principle from the Central Limit Theorem, of interest in U-statistics. The main contribution concerns convergence in total variation distance, using an abstract variant of Malliavin calculus for general random variables which verify a Doeblin type condition.

• Convergence in distribution norms in the Central Limit Theorem and Edgworth expansions [39] (V. Bally, L. Caramellino and G. Poly).

The convergence in "distribution norms" represents an extension of the convergence in total variation distance which permits to take into account some singular phenomenons. The main tool is the abstract Malliavin calculus mentioned above. Several examples are given in the paper and an outstanding application concerns the estimates of the number of roots of trigonometric polynomials. considered in a second paper; see [40].

• Bolzmann equation and Piecewise Deterministic Markov Processes. (see [41], [37]). In collaboration with D. Goreac and V. Rabiet, V. Bally has studied the regularity of the semigroup of *PDMP's* and, as an application estimates of the distance between two such semigroups. An interesting example is given by the two dimensional homogeneous Bolzmann equation. Furthermore, V. Bally obtained some exponential estimates for the function solution of this equation.

# **TOSCA Project-Team**

# 7. New Results

## 7.1. Probabilistic numerical methods, stochastic modelling and applications

**Participants:** Mireille Bossy, Nicolas Champagnat, Quentin Cormier, Madalina Deaconu, Olivier Faugeras, Coralie Fritsch, Pascal Helson, Antoine Lejay, Radu Maftei, Victor Martin Lac, Hector Olivero-Quinteros, Paolo Pigato, Denis Talay, Etienne Tanré, Milica Tomašević, Denis Villemonais.

#### 7.1.1. Published works and preprints

- M. Bossy, R. Maftei and Jean-François Jabir (National Research University Higher School of Economics, Moscow) propose and analyze the convergence of a time-discretization scheme for the motion of a particle when its instantaneous velocity is drifted by the known velocity of the carrying flow, and when the motion is taking into account the collision event with a boundary wall. We propose a symetrized version of the Euler scheme and prove a convergence of order one for the weak error. The regularity analysis of the associated Kolmogorov PDE is obtained by mixed variational and stochastic flow techniques for PDE problem with specular condition [46].
- N. Champagnat and B. Henry (IECL) studied a probabilistic approach for the Hamilton-Jacobi limit of non-local reaction-diffusion models of adaptive dynamics when mutations are small. They used a Feynman-Kac interpretation of the partial differential equation and large deviation estimates to obtain a variational characterization of the limit. They also studied in detail the case of finite phenotype space with exponentially rare mutations, where they were able to obtain uniqueness of the limit [48].
- N. Champagnat and P.-E. Jabin (Univ. Maryland) completed the study of the functional spaces in the article [18], devoted to the study of strong existence and pathwise uniqueness for stochastic differential equations (SDE) with rough coefficients, typically in Sobolev spaces.
- 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, defined as the original Markov process conditioned to never be absorbed. They prove that, under the conditions of [5], in addition to the uniform exponential convergence of the 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 → +∞. This allows them to obtain conditional ergodic theorems [22].
- N. Champagnat and D. Villemonais obtained criteria based on Lyapunov functions allowing to check the conditions of [5] which characterize the exponential uniform convergence in total variation of conditional distributions of an absorbed Markov process to a unique quasi-stationary distribution [50]. Among the various applications they give, they prove that these conditions apply to any logistic Feller diffusions in any dimension conditionned to the non extinction of all its coordinates. This question was left partly open since the first work of Cattiaux and Méléard on this topic [63].
- N. Champagnat and D. Villemonais obtained general conditions based on Foster-Lyapunov criteria
  ensuring the exponential convergence in total variation of the conditional distributions of an absorbed
  Markov process to a quasi-stationary distribution (QSD), with a speed that can depend on the initial
  distribution. In particular, these results provide a non-trivial subset of the domain of attraction of
  the minimal QSD of an absorbed process in cases where there is not uniqueness of a QSD. Similar
  results were only known for the very specific branching models. They also show how these criteria
  can be checked for a wide range of Markov processes in discrete or continuous time and in discrete

or continuous state spaces. In all these cases, they improve significantly the best known results. A particularly remarkable result is the existence of a principal eigenfunction for the generator of elliptic diffusion processes aborbed at the boundary of an open domain without any regularity assumption on the boundary of this domain [49].

- During his internship supervised by E. Tanré and R. Veltz (MATHNEURO Inria team), Q. Cormier studied numerically and theoretically a model of spiking neurons in interactions [51]. This model generalizes classical integrate and fire models: the neurons no more spike after hitting a deterministic threshold but spikes with a rate given as a function of the membrane potential (see e.g. [64]). He showed existence and uniqueness of the corresponding limit equation, and was able to extend those results in the case of excitatory and inhibitory neurons. He is now studying the long time behavior of the model, as part of his thesis.
- M. Deaconu and S. Herrmann studied the simulation of the hitting time of some given boundaries for Bessel processes. These problems are of great interest in many application fields as finance and neurosciences. More precisely they obtained recently a new method for the simulation of hitting times for Bessel processes with a non integer dimension. The main idea is to consider the simulation of the hitting time of Bessel processes with integer dimension and provide a new algorithm by using the additivity property of the laws of squared Bessel processes [26].
- M. Deaconu and S. Herrmann studied the Initial-Boundary Value Problem for the heat equation [25]. They construct an algorithm based on a random walk on heat balls in order to approximate the solution. Even if it represents a sophisticated 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 particular mean value formula for the heat equation and they obtained also a probabilistic formulation of this formula. They proved convergence results for this algorithm and illustrate them by numerical examples.
- M. Deaconu, S. Herrmann and S. Maire [27] introduced a new method for the simulation of the exit time and position of a δ-dimensional Brownian motion from a domain. The main interest of this method is that it avoids splitting time schemes as well as inversion of complicated series. The idea is to use the connexion between the δ-dimensional Bessel process and the δ-dimensional Brownian motion thanks to an explicit Bessel hitting time distribution associated with a particular curved boundary. This allows to build a fast and accurate numerical scheme for approximating the hitting time.
- M. Deaconu, B. Dumortier and E. Vincent (EPI Multispeech) are working with the Venathec SAS on the acoustic control of wind farms. Wind turbine noise is often annoying for humans living in close proximity to a wind farm. Reliably estimating the intensity of wind turbine noise is a necessary step towards quantifying and reducing annoyance, but it is challenging because of the overlap with background noise sources. Current approaches involve measurements with on/off turbine cycles and acoustic simulations, which are expensive and unreliable. This raises the problem of separating the noise of wind turbines from that of background noise sources and coping with the uncertainties associated with the source separation output. In their work they propose to assist a black-box source separation system with a model of wind turbine noise emission and propagation in a recursive Bayesian estimation framework. This new approach is validated on real data with simulated uncertainties using different nonlinear Kalman filters [38].
- M. Deaconu is working with L. Beznea and O. Lupaşcu (Bucharest, Romania) on the stochastic interpretation of rupture phenomena. They constructed a stochastic differential equation and a branching process for the fragmentation model. The main physical model involved in their study is the avalanche one and their model includes physical properties of the phenomenon. They introduced a new numerical algorithm issued from this study, which captures the fractal property of the avalanche [43].
- C. Fritsch, F. Campillo (Inria Sophia-Antipolis, MATHNEURO team) and O. Ovaskainen (Univ. Helsinki) proposed a numerical approach to determine mutant invasion fitness and evolutionary

singular strategies using branching processes and integro-differential models in [31]. They illustrate this method with a mass-structured individual-based chemostat model.

- P. Helson, E. Tanré and R. Veltz (MATHNEURO Inria team), have numerically and theoretically studied a model of spiking neurons in interaction with stochastic plasticity. A slow-fast analysis enabled to split the dynamic in two inhomogeneous Markov chains: one models the slow variable, the other one the fast variable. The jump rates of the slow chain is governed by the invariant distribution of the fast one. In his PhD thesis, P. Helson has proved existence and uniqueness of solution. Simple conditions for the slow variable to be recurrent and transient are given [53].
- A. Lejay, L. Lenôtre (CMAP, École Polytechnique) and G. Pichot (Inria Paris, SERENA team) have continued their work on the simulation of processes on discontinuous media [55]. A new Monte Carlo scheme, called the exponential timestepping scheme and based on closed form expression of the resolvent, is being studied.
- A. Lejay, E. Mordecki (U. de la República, Uruguay) and S. Torres (U. de Valparaíso, Chile) have continuous their work on the estimation of the parameter of the Skew Brownian motion [56].
- A. Lejay and P. Pigato have studied the estimation of the parameter of the Oscillating Brownian motion, which is a solution of a stochatic differential equation whose diffusivity takes two values [35].
- A. Lejay have given an alternative proof of the Girsanov theorem which is based on semigroups [39].
- In [60] D. Talay and M. Tomašević propose a new type of stochastic interpretation of the parabolicparabolic Keller-Segel systems. It involves an original type of McKean-Vlasov interaction kernel. At the particle level, each particle interacts with all the past of each other particle. At the mean-field level studied here, the McKean-Vlasov limit process interacts with all the past time marginals of its probability distribution. They prove that the one-dimensional parabolic-parabolic Keller-Segel system in the whole Euclidean space and the corresponding McKean-Vlasov stochastic differential equation are well-posed for any values of the parameters of the model.
- In collaboration with Jean-François Jabir (National Research University Higher School of Economics, Moscow) D. Talay and M. Tomašević prove the well–posedness of an original singularly interacting stochastic particle system associated to the one-dimensional parabolic-parabolic Keller-Segel model. They also establish the propagation of chaos towards this model [54].
- In [44] J. Bion-Nadal (Ecole Polytechnique) and D. Talay have introduced a Wasserstein-type distance on the set of the probability distributions of strong solutions to stochastic differential equations. This new distance is defined by restricting the set of possible coupling measures. They proved that it may also be defined by means of the value function of a stochastic control problem whose Hamilton–Jacobi–Bellman equation has a smooth solution, which allows one to deduce a priori estimates or to obtain numerical evaluations. They have exhibited an optimal coupling measure and characterized it as a weak solution to an explicit stochastic differential equation, and they finally have described procedures to approximate this optimal coupling measure.

A notable application concerns the following modeling issue: given an exact diffusion model, how to select a simplified diffusion model within a class of admissible models under the constraint that the probability distribution of the exact model is preserved as much as possible?

- E. Tanré has worked with Patricio Orio (CINV, Chile) and Alexandre Richard (Centrale-Supelec) on the modelling and measurement of long-range dependence in neuronal spike trains. They exhibit evidence of memory effect in genuine neuronal data and compared a fractional integrate-and-fire model with the existing Markovian models (paper in revision: [59]).
- D. Villemonais worked with his Research Project student William Oçafrain (École des Mines de Nancy) on an original mean-field particle system [36]. 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.

- D. Villemonais, Camille Coron (Université Paris XI) and Sylvie Méléard (École Polytechnique) proved a criterion for the integrability of paths of one-dimensional diffusion processes in [52] from which we derive new insights on allelic fixation in several situations.
- D. Villemonais obtains a lower bound for the coarse Ricci curvature of continuous time pure jump Markov processes in [61], with an emphasis on interacting particle systems. In this preprint, several models are studied, with a detailed study of the herd behavior of a simple model of interacting agents. The lower bound is shown to be sharp for birth and death processes.

### 7.1.2. Other works in progress

- M. Bossy, J. Fontbona (Universidad de Chile, Chile) and H. Olivero-Quinteros are working in a model for a network of neurons interacting electrically and chemically in a mean field fashion. They have proved the synchronization of the network under suitable values for the parameters of the model and a concentration result for the mean field limit.
- N. Champagnat is working with P. Vallois (IECL and Inria BIGS team) and L. Vallat (CHRU Strasbourg) on the inference of dynamical gene networks from RNAseq and proteome data.
- N. Champagnat, C. Fritsch and S. Billiard (Univ. Lille) are working on food web modeling.
- N. Champagnat, C. Fritsch and D. Villemonais are working with A. Gégout-Petit, P. Vallois, A. Mueller-Gueudin (IECL and Inria BIGS team), A. Kurtzmann (IECL), A. Harlé, J.-L. Merlin (ICL and CRAN) and E. Pencreac'h (CHRU Strasbourg) within an ITMO Cancer project on modeling and parametric estimation of dynamical models of circulating tumor DNA (ctDNA) of tumor cells, divided into resistant and sensitive ctDNA depending on whether they hold mutations known to provide resistance to a given targeted therapy or not. The goal of the project is to predict sooner and more accurately the emergence of resistance to the targeted therapy in a patient's tumor, so that the patient's therapy can be modulated more efficiently.
- M. Deaconu and S. Herrmann are working on numerical approaches for hitting times of some general stochastic differential equations.
- M. Deaconu, O. Lupaşcu and L. Beznea (Bucharest, Romania) are working on the connexion between branching processes and partial differential equations in fluid mechanics.
- M. Deaconu, B. Dumortier and E. Vincent (EPI Multispeech) are working on handling uncertainties in the wind farms model in order to design a stochastic algorithm.
- M. Deaconu and R. Stoica (Université de Lorraine, Nancy) are working on the ABC Shadow algorithm and its possible generalizations.
- O. Faugeras, E. Soret and E. Tanré are working on Mean-Field descriptions or thermodynamics limits of large populations of neurons. They study a system of EDS which describes the evolution of membrane potential of each neuron over the time when the synaptic weights are random variables (not assumed to be independent).
- O. Faugeras, James Maclaurin (Univ. of Utah) and E. Tanré have worked on the asymptotic behavior of a model of neurons in interaction with correlated gaussian synaptic weights. They have obtained the limit equation as a singular non-linear SDE and a Large Deviation Principle for the law of the finite network.
- 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.
- P. Helson, E. Tanré and R. Veltz (MATHNEURO Inria team) are working on a mathematical framework for plasticity models. The aim is to propose a 'optimized' model of memory capacity and memory lifetime.
- A. Lejay, A. Brault (Univ. Toulouse) and L. Coutin (Univ. Toulouse) are working on a non linear generalization of the sewing lemma, which is the main technical tool in the theory of rough paths.

- V. Martin Lac, H. Olivero-Quinteros and D. Talay are working on theoretical and algorithmic questions related to the simulation of large particle systems under singular interactions and to the simulation of independent random variables with heavy tails.
- C. Graham (École Polytechnique) and D. Talay are ending and polishing the second volume of their series on Mathematical Foundation of Stochastic Simulation to be published by Springer.
- P-E. Jabin (University of Maryland) and D. Talay are working on a mean-field game and developing a new technique to analyse it.
- E. Tanré is working with Nicolas Fournier (Univ. Pierre et Marie Curie, Paris 6) and Romain Veltz (MATHNEURO Inria team) on a network of spiking networks with propagation of spikes along the dendrites. Consider a large number n of neurons randomly connected. When a neuron spikes at some rate depending on its electric potential, its potential is set to a minimum value v<sub>min</sub>, and this makes start, after a small delay, two fronts on the dendrites of all the neurons to which it is connected. Fronts move at constant speed. When two fronts (on the dendrite of the same neuron) collide, they annihilate. When a front hits the soma of a neuron, its potential is increased by a small value w<sub>n</sub>. Between jumps, the potentials of the neurons are assumed to drift in [v<sub>min</sub>, ∞), according to some well-posed ODE. We prove the existence and uniqueness of a heuristically derived mean-field limit of the system when n → ∞.
- E. Tanré is working with Alexandre Richard (Centrale-Supelec) and Soledad 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 of the Hurst parameter H of the noise (fBM) is larger than 0.5. 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.
- D. Villemonais works in collaboration with Éliane Albuisson (CHRU of Nancy), Athanase Benetos (CHRU of Nancy), Simon Toupance (CHRU of Nancy), Daphné Germain (École des Mines de Nancy), Anne Gégout-Petit (Inria BIGS team) and Sylvain Chabanet (École des Mines de Nancy). The aim of this collaboration is to conduct a statistical study of the time evolution of telomere's length in human cells.
- D. Villemonais started a collaboration with Cécile Mailler (University of Bath) with the aim of studying the almost sure convergence of measure valued Pólya urns models.

## **7.2. Financial Mathematics**

Participants: Madalina Deaconu, Antoine Lejay, Paolo Pigato, Khaled Salhi, Etienne Tanré.

#### 7.2.1. Published works and preprints

- When the underlying asset price is given by a exponential Lévy model, the market is almost incomplete. Under this hypothesis, M. Deaconu, A. Lejay and K. Salhi worked 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 [28].
- A. Lejay and P. Pigato studied the estimation of the coefficients of the Geometric Oscillating Brownian motion on financial data. This stochastic process is a modification of the Black & Scholes model that takes into account leverage effect and other sudden changes in the volatility [57], [41].
- V. Reutenauer and E. Tanré have worked on extensions of the exact simulation algorithm introduced by Beskos et al. [62]. 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 onedimensional diffusion process and  $\Psi$  any test-function. They also propose an efficient modification of Beskos et al. algorithm ([58], paper in revision).