RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2018

Section New Results

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ACUMES Project-Team

7. New Results

7.1. Macroscopic traffic flow models on networks

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The relaxation limit for ARZ model. The Aw-Rascle-Zhang model [55], [157] can now be considered as a classical traffic flow model. In [27], we detail the mathematical behavior of the Aw-Rascle-Zhang model with relaxation [54]. In a Lagrangian setting, we use the Wave-Front-Tracking method with splitting technique to construct a sequence of approximate solutions. We prove that this sequence admits a limit. We then show that the limit is a weak entropy solution of the relaxed system associated to a given initial datum with bounded variation. Finally, we prove that this limit converges to a weak solution of the scalar conservation law when the relaxation parameter goes to zero.

Bounded acceleration. In [29], 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.

Second order models with moving bottlenecks. In [25], we study the Aw-Rascle-Zhang (ARZ) model with non-conservative local point constraint on the density flux introduced in [Garavello, M., and Goatin, P. The Aw-Rascle traffic model with locally constrained flow. Journal of Mathematical Analysis and Applications 378, 2 (2011), 634-648], its motivation being, for instance, the modeling of traffic across a toll gate. We prove the existence of weak solutions under assumptions that result to be more general than those required in [Garavello, M., and Villa, S. The Cauchy problem for the Aw-Rascle-Zhang traffic model with locally constrained flow. Journal of Hyperbolic Differential Equations 14, 03 (2017), 393-414]. More precisely, we do not require that the waves of the first characteristic family have strictly negative speeds of propagation. The result is achieved by showing the convergence of a sequence of approximate solutions constructed via the wave-front tracking algorithm. The case of solutions attaining values at the vacuum is considered. We also present an explicit numerical example to describe some qualitative features of the solutions.

Traffic control by autonomous vehicles. We consider the possibility of properly controlling a moving bottleneck to improve the traffic flow. 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 [30] the MPC (Model Predictive Control) approach is used 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.

Well-posedness of conservation laws on networks with finite buffers. In collaboration with A. Bayen and A. Keimer (UC Berkeley), we introduce a model capable of dealing with conservation laws on networks and the coupled boundary conditions at the junctions. To that end we introduce a buffer of fixed arbitrary size and time dependent split ratios at the junctions which represent how traffic should be routed. One of the most important and interesting property of the presented model is its capability of showing spill-back phenomena over junctions. Having defined the dynamics on the level of conservation laws we lift them up to Hamilton Jacobi equations. The corresponding formulation in terms of H-J allows us to attack the problem that boundary datum of in and out-going junctions is a function of the queue size and vice versa. We do this by defining a fixed-point problem in a proper Banach space setting and prove the existence of a solution. Thus, the problem is solved on the level of Hamilton-Jacobi equations and due to the existent theory we also obtain a solution on the level of conservation laws with boundary datum in the sense of Bardos-Leroux-Nédélec.

Altogether, the system of conservation laws – locally coupled via the boundary conditions is studied for analytical questions of well-posedness, uniqueness and existence.

Finally we detail how to use this framework on a non-trivial road network, with several intersections and finite-length links.

Minimum time boundary controls. In collaboration with A. Bayen and A. Keimer (UC Berkeley), we are investigating the minimum time control problem for traffic flow. More precisely, we seek for the inflow upstream boundary condition that drives congested traffic to free flow condition on a stretch of road in minimum time.

Big Data analysis and modeling of road Traffic. Yunzhi Wu's internship, funded by Inria under the program "Transverse Actions", was co-supervised by Acumes (P. Goatin and G. Costeseque) and Zenith (F. Masseglia and R. Akbarinia). In this project, we processed the traffic data collected by loop detectors in the Mediterranean region during 3 months in 2015 (provided by DIRMED). We aimed at finding out the characteristics of traffic data and provide a new way of traffic prediction and estimation. The method of Motif Discovery was used for abnormality detection and pattern discovery. A modified method was also used for congestion prediction. Then we use the Co-Clustering method to group the data by day and loop. The clustering results were used to do a grouped calibration of fundamental diagram.

7.2. Non-local conservation laws

Participants: Felisia Angela Chiarello, Paola Goatin, Elena Rossi, Florent Berthelin [COFFEE, Inria].

F.A. Chiarello's PhD thesis focuses on non-local conservation laws. In [22], we proved the stability of entropy weak solutions, considering smooth kernels. We obtained an estimate on the dependence of the solution with respect to the kernel function, the speed and the initial datum, applying the doubling of variables technique. We also provided some numerical simulations illustrating the dependencies above for some cost functionals derived from traffic flow applications.
In the paper [21], we proved the existence for small times of weak solutions for a class of non-local systems in one space dimension, arising in traffic modeling. We approximated the problem by a Godunov type numerical scheme and we provided uniform L^∞ and BV estimates for the sequence of approximate solutions. We showed some numerical simulations illustrating the behavior of different classes of vehicles and we analyzed two cost functionals measuring the dependence of congestion on traffic composition.
We also conducted a study on Lagrangian-Antidiffusive Remap schemes (previously proposed for classical hyperbolic systems) for the above mentioned non-local multi-class traffic flow model. The error and convergence analysis show the effectiveness of the method, which is first order, in sharply capturing shock discontinuities, and better precision with respect to other methods as Lax-Friedrichs or Godunov (even 2nd order). A journal article about these results is submitted [40].

In the setting of Florent Berthelin's secondement, we studied the regularity properties of solutions of a non-local traffic model involving a convolution product. Unlike other studies, the considered kernel is discontinuous on $\mathbb{R}$. We proved Sobolev estimates and the convergence of approximate solutions solving a viscous and regularized non-local equation. It leads to weak, $C([0,T],L^2(\mathbb{R}))$, and smooth, $W^{2,2N}([0,T]\times\mathbb{R})$, solutions for the non-local traffic model [16].

7.3. Well-posedness results for Initial Boundary Value Problems

Participants: Paola Goatin, Elena Rossi.

We focused on the IBVP for a general scalar balance law in one space dimension and proved its well-posedness and the stability of its solutions with respect to variations in the flux and in the source terms. For both results, the initial and boundary data are required to be bounded functions with bounded total variations. The existence of solutions is obtained from the convergence of a Lax-Friedrichs type algorithm, while the stability follows from an application of Kruzkov's doubling of variables method [33].

Exploiting the same techniques, we focused also on a non local version of the scalar IBVP for a conservation law. The flux is indeed assumed to depend non locally on the unknown, and the non local operator is "aware of boundaries". For this non local problem, existence and uniqueness of solutions are provided. In particular, the uniqueness follows from the Lipschitz continuous dependence on initial and boundary data, which is proved exploiting the results on the local IBVP [43].

7.4. Isogeometric analysis

Participants: Régis Duvigneau, Stefano Pezzano, Maxime Stauffert, Asma Azaouzi [ENIT], Maher Moakher [ENIT].

High-order isogeometric solvers are developed, based on CAD representations for both the geometry and the solution space, for applications targeted by the team, in particular hyperbolic or convection-dominated problems. Specifically, we investigate a Discontinuous Galerkin method for hyperbolic systems such as compressible Euler, or Navier-Stokes equations, based on an isogeometric formulation[24]: 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) thanks to Bézier extraction techniques, while the same rational approximation space is adopted for the solution.

This topic has been studied in the context of A. Azaouzi's PhD work defended in December 2018, in co-supervision with M. Moakher at ENIT. Current works concern local refinement strategies by splitting algorithms, the arbitrary Lagrangian-Eulerian formulation in the isogeometric context (PhD work of S. Pezzano) and high-order shape sensitivity analysis (Post-doc of M. Stauffert, PRE "GeoSim").

7.5. Sensitivity equation method for hyperbolic systems

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

While the sensitivity equation method is a common approach for parabolic systems, its use for hyperbolic ones is still tedious, because of the generation of discontinuities in the state solution, yielding Dirac distributions in the sensitivity solution. To overcome this difficulty, we investigate a modified sensitivity equation, that includes an additional source term when the state solution exhibits discontinuities, to avoid the generation of delta-peaks in the sensitivity solution. We consider as 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[18].

This study is achieved in collaboration with C. Chalons from University of Versailles, in the context of C. Fiorini's PhD work, defended in July 2018.

7.6. 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[35].

The method is applied to the optimization of foils and sails in the context of racing yachts[34], in particular for the America's Cup in collaboration with Groupama team. This work was part of M. Sacher's PhD work at Ecole Navale, defended in September 2018.

7.7. Solving with games the coupled problems 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].

We extend in two directions our previous successful attempts [112], [121] to tackle ill posed inverse problems as Nash games.

In a first direction, a Nash game algorithm is used for the solution of coupled conductivity identification and data completion in cardiac electrophysiology. In [19], we consider the identification problem of the conductivity coefficient for an elliptic operator using an incomplete over-specified measurements on the surface. We define three players with three corresponding criteria. The two first players use Dirichlet and Neumann strategies to solve the completion problem, while the third one uses the conductivity coefficient as strategy, and uses a cost which basically relies on an established identifiability theorem. The implemented algorithm is used for the electrocardiography ECG imaging inverse problem, dealing with inhomogeneities in the torso domain. The inverse problem of ECG consists in finding the electric potential distribution on the heart's surface given the one on the torso, so that it is a data completion problem. Furthermore, in our approach, the conductivity coefficients are known only by an approximate values. we conduct numerical experiments on a 2D torso case including noisy measurements. Results illustrate the ability of our computational approach to tackle the difficult problem of joint identification and data completion.

The second direction deals with Nash strategies for the inverse inclusion Cauchy-Stokes problem. We introduce in [44] a new algorithm to solve the problem of detecting unknown cavities immersed in a stationary viscous fluid, using partial boundary measurements. The considered fluid obeys a steady Stokes regime, the cavities are inclusions and the boundary measurements are a single compatible pair of Dirichlet and Neumann data, available only on a partial accessible part of the whole boundary. This inverse inclusion Cauchy-Stokes problem is ill-posed for both the cavities and missing data reconstructions, and designing stable and efficient algorithms is not straightforward. We reformulate the problem as a three-player Nash game. Thanks to an identifiability result derived for the Cauchy-Stokes inclusion problem, it is enough to set up two Stokes BVP, then use them as state equations. The Nash game is then set between 3 players, the two first targeting the data completion while the third one targets the inclusion detection. We used a level-set approach to get rid of the tricky control dependence of functional spaces, and we provided the third player with the level-set function as strategy, with a cost functional of Kohn-Vogelius type. We propose an original algorithm, which we implemented using Freefem++. We present 2D numerical experiments for three different test-cases.The obtained results corroborate the efficiency of our 3-player Nash game approach to solve parameter or shape identification for Cauchy problems.

7.8. The Kalai-Smorodinski solution for many-objective Bayesian optimization

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

Game theory finds nowadays a broad range of applications in engineering and machine learning. However, in a derivative-free, expensive black-box context, very few algorithmic solutions are available to find game equilibria. In [31], we propose a novel Gaussian-process based approach for solving games in this context. We follow a classical Bayesian optimization framework, with sequential sampling decisions based on acquisition functions. Two strategies are proposed, based either on the probability of achieving equilibrium or on the Stepwise Uncertainty Reduction paradigm. Practical and numerical aspects are discussed in order to enhance the scalability and reduce computation time. Our approach is evaluated on several synthetic game problems with varying number of players and decision space dimensions. We show that equilibria can be found reliably for a fraction of the cost (in terms of black-box evaluations) compared to classical, derivative-based algorithms.

Another ongoing scope of research in multi-objective Bayesian optimization is to extend its applicability to a large number of objectives : the so-called many-objective optimization. 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-Smorodinsky solution, that possesses attractive properties. In particular, it ensures equal marginal gains over all objectives. We further make it insensitive to a monotonic transformation of the objectives by considering the objectives in the copula space. A novel tailored algorithm is proposed to search for the solution, in the form of a Bayesian optimization algorithm: sequential sampling decisions are made based on acquisition functions that derive from an instrumental GP prior. Our approach is tested on three problems with respectively four, six and ten objectives.

The Nash and Kalai-Smorodinsky methods are available in the R package `GPGame` available on CRAN at https://cran.r-project.org/package=GPGame.

7.9. Stochastic multiple gradient descent algorithm

Participants: Jean-Antoine Désidéri, Fabrice Poirion [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.], Quentin Mercier [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.].

We have proposed a new method for multi-objective optimization problems in which the objective functions are expressed as expectations of random functions. The present method is based on an extension of the classical stochastic gradient algorithm and a deterministic multi-objective algorithm, the Multiple Gradient Descent Algorithm (MGDA). In MGDA a descent direction common to all specified objective functions is identified through a result of convex geometry. The use of this common descent vector and the Pareto stationarity definition into the stochastic gradient algorithm makes the algorithm able to solve multi-objective problems. The mean square and almost sure convergence of this new algorithm are proven considering the classical stochastic gradient algorithm hypothesis. The algorithm efficiency is illustrated on a set of benchmarks with diverse complexity and assessed in comparison with two classical algorithms (NSGA-II, DMS) coupled with a Monte Carlo expectation estimator [129]

7.10. Non-convex multiobjective optimization under uncertainty

Participants: Jean-Antoine Désidéri, Fabrice Poirion [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.], Quentin Mercier [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.].

A novel algorithm for solving multi-objective design optimization problems with non-smooth objective functions and uncertain parameters is presented. The algorithm is based on the existence of a common descent vector for each sample of the random objective functions and on an extension of the stochastic gradient algorithm. The proposed algorithm is applied to the optimal design of sandwich material. Comparisons with the genetic algorithm NSGA-II and the DMS solver are given and show that it is numerically more efficient due to the fact that it does not necessitate the objective function expectation evaluation. It can moreover be entirely parallelized. Another simple illustration highlights its potential for solving general reliability problems, replacing each probability constraint by a new objective written in terms of an expectation. Moreover, for this last application, the proposed algorithm does not necessitate the computation of the (small) probability of failure [129].

CAGIRE Project-Team

7. New Results

7.1. A density-based flux scheme scheme for simulating low Mach flows

Participants: Pascal Bruel, Jonathan Jung, Vincent Perrier.

The topic dealt with concerns acoustic computations in low Mach number flows with density based solvers. For ensuring a good resolution of the low Mach number base flow, a scheme able to deal with stationary low Mach number flows is necessary. Previously proposed low Mach number fixes have been tested with acoustic computations. Numerical results prove that they are not accurate for acoustic computations. The issues raised with acoustic computations with low Mach number fixes were studied and a new scheme has been developed, in order to be accurate not only for steady low Mach number flows, but also for acoustic computations. Numerical tests evidenced the improvement of the proposed scheme with respect to the state of the art [9].

7.2. A parameter free pressure based approach for simulating flows at all Mach

Participant: Pascal Bruel.

A pressure-correction algorithm developed in close partnership with Prof. E. Dick (Ghent University, Belgium) and Dr. Y. Moguen (UPPA, France) has been developed and extensively tested for a wide range of compressible fluid flow regimes. It proved to be well-suited to simulate flows at all levels of Mach number with smooth and discontinuous flow field changes, by providing a precise representation of convective transport and acoustic propagation. A co-located finite volume space discretization is used with the AUSM flux splitting. It is demonstrated that two ingredients are essential for obtaining good quality solutions: the presence of an inertia term in the transporting velocity expression; a velocity difference diffusive term in the face pressure expression, with a correct Mach number scaling to recover the hydrodynamic and acoustic low Mach number limits. To meet these two requirements, a new flux scheme, named MIAU, for Momentum Interpolation with Advection Upstream splitting has been proposed (one journal paper submitted in 2018).

7.3. New models for conjugate heat transfer

Participant: Rémi Manceau.

New models valid in the near-wall region have been proposed for both the turbulent heat flux and the dissipation rate of the temperature variance in the framework of the EDF CIFRE PhD thesis of G. Mangeon. The purpose is to extend the Elliptic Blending approaches developed in the team to all possible boundary conditions for the temperature: imposed wall-temperature, imposed heat flux or conjugate heat transfer, which is of primary importance for applications in the nuclear industry. The new full model (which associates the two above-mentioned models) is the first one to satisfy all the near-wall budgets and, consequently, the asymptotic behavior of all the quantities. These results have been presented at two international symposia [16], [15].

CARDAMOM Project-Team

7. New Results

7.1. Modelling of free surface flows

- Participants: Umberto Bosi, Mathieu Colin, Maria Kazolea, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

This year we have continued our work on Boussinesq-type models. We have focused on the enhanced equations of Nwogu [101], and on a frequency enhanced version of the Green-Naghdi system as proposed in [55], [77]. These models allow to account for weak dispersive effects which become relevant in the near shore region. Two papers on the topic are published. The first one [9] compares two popular wave breaking closures. We perform a study of the behaviour of the two closures for different mesh sizes, with attention to the possibility of obtaining grid independent results. Based on a classical shallow water theory, we also suggest some monitors to quantify the different contributions to the dissipation mechanism, differentiating those associated to the scheme from those of the partial differential equation. Our main results show that numerical dissipation contributes very little to the the results obtained when using eddy viscosity method. This closure shows little sensitivity to the grid, and may lend itself to the development and use of non-dissipative/energy conserving numerical methods. The opposite is observed for the hybrid approach, for which numerical dissipation plays a key role, and unfortunately is sensitive to the size of the mesh. The second paper [8] presents the application and validation, with respect to the transformation, breaking and run-up of irregular waves, of an unstructured high-resolution finite volume (FV) numerical solver for the 2D extended BT equations of [101].

The extension of these techniques to also account for the presence of floating structures is ongoing [34].
The methods and models developed have also led to physical studies and applications. In particular, in collaboration with the EPOC laboratory in Bordeaux, we are conducting a parametric study of bore propagation in estuaries. In particular, Three types of bores are observed in nature long wavelength undulating, short wavelength undulating, and breaking. The first kind is invisible to the eye, but measurable. The other two can be seen during mascarets. Understanding the mechanisms ruling the transition from one to the other has tremendous impact on human activities in estuarine areas. We introduced a new set of dimensionless parameters to characterize the transition to breaking bores. We have shown that they allow to determine if the transition is dominated by friction or nonlinearity (wave amplitude). The work discussed in [7] somewhat represents an accomplishment of our activity, combining simulations using fully non-linear unstructured grid dispersive models, an exploration of parameter space based on adaptive sampling, locally enriched using a smoothness indicator related to the onset of wave breaking. Further extensions of this work are ongoing, and aim at proposing some mechanism for the first transition (see the preprint [35]).

7.2. Modelling of icing and de-icing of aircrafts

- Participants: Heloise Beaugendre, Mathieu Colin and Francois Morency
- Corresponding member: Heloise Beaugendre

Flying debris is generated in several situations: when a roof is exposed to a storm, when ice accretes on rotating wind turbines, or during inflight aircraft deicing. Four dimensionless parameters play a role in the motion of flying debris. The goal of our work was to investigate the relative importance of four dimensionless parameters: the Reynolds number, the Froude number, the Tachikawa number, and the mass moment of inertia parameters. Flying debris trajectories have been computed with a

fluid-solid interaction model formulated for an incompressible 2D laminar flow. The rigid moving solid effects are modelled in the Navier-Stokes equations using penalization. A VIC scheme was used to solve the flow equations. The aerodynamic forces and moments are used to compute the acceleration and the velocity of the solid. A database of 64 trajectories has been built using a two-level full factorial design for the four factors. The dispersion of the plate position at a given horizontal position decreases with the Froude number. Moreover, the Tachikawa number has a significant effect on the median plate position.
Ice release is of concern to aircraft manufacturers due to the potential damage that the ice debris can cause on aircraft components. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. High-fidelity models involve fully coupled time-accurate aerodynamic and flight mechanics simulations and thus require the use of emerging simulation tools, such as approaches based on immersed boundary methods or chimera grids. The developments of current simulations tools for ice block trajectories performed in the scope of the recently completed research project STORM have been described and validated against a STORM experimental data base of trajectories created by the German Aerospace Center (DLR) in collaboration with the German-Dutch Wind Tunnel foundation.
Immersed boundary methods (IBM) are alternative methods to simulate fluid flows around complex geometries. The grid generation is fast as it does not need to conform to the fluid-solid interface. However, special treatments are needed in the flow equations to properly take into account the wall proximity. The penalization method is a particular case of the IBM in which the wall boundary conditions are imposed via continuous forcing terms into the governing equations. Reynolds Averaged NavierâStokes (RANS) equations completed with a turbulence model are still the most common way to model turbulence in engineering applications. However, RANS turbulence model implementation with penalization into a vortex formulation is not straight forward, in part because of the variable turbulent viscosity and partly because of the boundary conditions. Our work extends the penalization technique to turbulent flows. The objective is to validate the use of the SpalartâAllmaras turbulence model in the context of penalization and vortex formulation. Details of the resolution using a Vortex In Cell (VIC) numerical scheme are given. The proposed scheme is based on the advection of particles of vorticity and particles of turbulent viscosity. A Lagrangian framework is chosen to solve the advection part. The remaining parts of the system of equations are solved with an Eulerian framework using a Cartesian uniform grid. To avoid fine meshes near the wall, a wall function compatible with the penalization method and the vortex formulation is proposed. The formulation and the coding are validated against the wellknown periodic channel flow. Velocity profiles are computed without and with the wall function. Results agree with analytic law of the wall solutions, showing that RANS simulations can be conducted with VIC schemes and penalization.
Ice formation can reduce the efficiency of aircraft lifting surfaces. Experiments proved that even the onset of icing (increased roughness) could cause an increase of 63% on the minimum drag coefficient of a NACA0015 airfoil when compared to a smooth airfoil. To investigate stall behavior due to ice formation, a roughness wall extension for the Spalart-Allmaras turbulence model was implemented in the open-source code SU2 so that the onset of ice formation could also be evaluated.

7.3. High order embedded and immersed boundary methods

- Participants: Heloise Beaugendre and Mario Ricchiuto
- Corresponding member: Heloise Beaugendre

Immersed and embedded methods are a flexible and efficient approach to handle complex, and moving geometries. In these techniques, domain boundaries are not meshed exactly, but are embedded/immersed in the grid. Ad-hoc techniques are then required to account for the effect of the coupling/boundary conditions defined on the domain boundaries on the nodes in the computational domain. This year we have made some progress on these methods on two aspects.
Preliminary results on the use of higher order schemes with penalization have been obtained. As in [100], the main idea is to combine a simple penalization technique to impose the no-slip condition

with mesh adaptation to control the error. In the work done this year we have looked into the possibility of exploiting curved meshes and higher order schemes to further improve the accuracy in laminar flow computations [20], [21].

In parallel, we have worked on a different strategy to achieve higher order in the context of an embedded approach: the shifted boundary method, initially proposed in [92], [93]. We have worked on an extension of this method to hyperbolic problems, which are difficult to treat with penalization. The extension proposed for linear waves, as well as for the nonlinear shallow water equations show that second order results can be easily achieved in this context [15] (see also [27], [26]).

7.4. Adaptation techniques

- Participants: Heloise Beaugendre, Cecile Dobrzynski and Mario Ricchiuto
- Corresponding member: Cecile Dobrzynski
  Previous work on interpolation free adaptation for compressible flows [107] has been further extended to account for non-ideal gas effects. Simulations are carried out to assess grid adaptation criteria in presence of these effects [12]. We have found that for some cases, especially in presence of a strong non-ideal dependence of the speed of sound on the density and the temperature, Mach number estimators prove to be more effective.
  We have also completed the study of adaptive mesh deformation for shallow water flows, and proposed a comprehensive study of the efficiency of different techniques based on a adapt-project-evolve paradigm, or on a fully coupled ALE approach. The issue of marrying mass conservation and well-balancedness, which is peculiar to shallow water models, has been treated by means of a high order projection of the topography [3]. Preliminary results on the extension of these techniques have also been obtained [16].

7.5. Composites Materials

- Participants: Mathieu Colin, Cecile Dobrzynski and Mario Ricchiuto
- Corresponding member: Mario Ricchuito

  We have continued our study on composite materials. We have finalized the phd of Xi Lin. We have finished to write the fluid models describing the propagation of an oxyde in the cracks appearing in self-healing composite materials. More precisely, we obtained two families of models, governed by the boundaries conditions. The first one looks like Shallow Water Equations and the second one comes from Lubrication theory. In order to evaluate the relevance of our models, we investigate the well-posedness of our model. In this direction, in [58] we propose in the full generality a link between the BD entropy introduced by D. Bresch and B. Desjardins for the viscous shallow-water equations and the Bernis-Friedman (called BF) dissipative entropy introduced to study the lubrications equations. Different dissipative entropies are obtained playing with the drag terms on the viscous shallow water equations. It helps for instance to prove global existence of nonnegative weak solutions for the lubrication equations starting from the global existence of nonnegative weak solutions for appropriate viscous shallow-water equations. Two articles are in preparation.

DEFI Project-Team

7. New Results

7.1. Qualitative and quantitative methods for inverse problems

7.1.1. On the Factorization Method for a Far Field Inverse Scattering Problem in the Time Domain

F. Cakoni, H. Haddar and A. Lechleiter

We develop a factorization method to obtain explicit characterization of a (possibly non-convex) Dirichlet scattering object from measurements of time-dependent causal scattered waves in the far field regime. In particular, we prove that far fields of solutions to the wave equation due to particularly modified incident waves, characterize the obstacle by a range criterion involving the square root of the time derivative of the corresponding far field operator. Our analysis makes essential use of a coercivity property of the solution of the Dirichlet initial boundary value problem for the wave equation in the Laplace domain. This forces us to consider this particular modification of the far field operator. The latter in fact, can be chosen arbitrarily close to the true far field operator given in terms of physical measurements.

7.1.2. New interior transmission problem applied to a single Floquet–Bloch mode imaging of local perturbations in periodic media

F. Cakoni, H. Haddar and T.P Nguyen

We consider the imaging of local perturbations of an infinite penetrable periodic layer. A cell of this periodic layer consists of several bounded inhomogeneities situated in a known homogeneous media. We use a differential linear sampling method to reconstruct the support of perturbations without using the Green's function of the periodic layer nor reconstruct the periodic background inhomogeneities. The justification of this imaging method relies on the well-posedeness of a nonstandard interior transmission problem, which until now was an open problem except for the special case when the local perturbation did not intersect the background inhomogeneities. The analysis of this new interior transmission problem is the main focus of this paper. We then complete the justification of our inversion method and present some numerical examples that confirm the theoretical behavior of the differential indicator function determining the reconstructable regions in the periodic layer.

7.1.3. A robust Expectation-Maximization method for the interpretation of small angle scattering data on dense nanoparticle samples

M. Bakry, H. Haddar and O. Bunau

The Local Monodisperse Approximation (LMA) is a two-parameters model commonly employed for the retrieval of size distributions from the small angle scattering (SAS) patterns obtained on dense nanoparticle samples (e.g. dry powders and concentrated solutions). This work features an original, beyond state-of-the-art implementation of the LMA model resolution for the inverse scattering problem. Our method is based on the Expectation Maximization iterative algorithm and is free from any fine tuning of model parameters. The application of our method on SAS data acquired in laboratory conditions on dense nanoparticle samples is shown to provide very good results.

7.1.4. Detecting Sound Hard Cracks in Isotropic Inhomogeneities

L. Audibert, L. Chesnel, H. Haddar and Kevish Napal

We consider the problem of detecting the presence of sound-hard cracks in a non homogeneous reference medium from the measurement of multi-static far field data. First, we provide a factorization of the far field operator in order to implement the Generalized Linear Sampling Method (GLSM). The justification of the analysis is also based on the study of a special interior transmission problem. This technique allows us to recover the support of the inhomogeneity of the medium but fails to locate cracks. In a second step, we consider a medium with a multiply connected inhomogeneity assuming that we know the far field data at one given frequency both before and after the appearance of cracks. Using the Differential Linear Sampling Method (DLSM), we explain how to identify the component(s) of the inhomogeneity where cracks have emerged. The theoretical justification of the procedure relies on the comparison of the solutions of the corresponding interior transmission problems without and with cracks. Finally we illustrate the GLSM and the DLSM providing numerical results in 2D. In particular, we show that our method is reliable for different scenarios simulating the appearance of cracks between two measurements campaigns

7.1.5. Uncertainty Analysis and Calibration of the Catalytic Properties of Thermal Protection Materials: Formulation of the Bayesian Inference Problem

P.M. Congedo, F. Sanson, T. Magin, F. Panerai

Quantifying the catalytic properties of reusable thermal protection system materials is essential for the design of atmospheric entry vehicles. Their properties quantify the recombination of oxygen and nitrogen atoms into molecules, and allow for accurate computation of the heat flux to the spacecraft. Their rebuilding from ground test data, however, is not straightforward and subject to uncertainties. We propose a fully Bayesian approach to reconstruct the catalytic properties of ceramic matrix composites from sparse high-enthalpy facility experimental data with uncertainty estimates. The results are compared to those obtained by means of an alternative reconstruction procedure, where the experimental measurements are also treated as random variables but propagated through a deterministic solver. For the testing conditions presented in this work, the contribution to the measured heat flux of the molecular recombination is negligible. Therefore, the material catalytic property cannot be estimated precisely. Moreover, epistemic uncertainties are rigorously included, such as the unknown reference calorimeter catalytic property.

7.1.6. A Bayesian framework for the investigation of complex fluid vapor flows

P.M. Congedo, G. Gori, O. Le Maitre, A. Guardone

The present work develops a Bayesian framework for the inference of complex fluid thermodynamic model parameters. The objective is to numerically assess the potential of using experimental measurements to reduce the aleatoric and epistemic uncertainties inherent the Peng-Robinson thermodynamic fluid model for flows of fluids in the non-ideal regimes. Our Bayesian framework is tailored to the design of the TROVA (Test-Rig for Organic VApors) experimental facility, at Politecnico di Milano. Computational Fluid Dynamics (CFD) simulations are used to predict the flow field within the designed test section whereas surrogate models (Polynomial-Chaos expansion) are constructed to account for the predictions dependence on the thermodynamic model parameters. First, synthetic data are generated in the attempt of reproducing a real test case, which is considered as the reference experiment, actually achieved in the TROVA facility. We investigate the resulting posterior uncertainties and assess the knowledge brought by using diverse type of measurements obtained for a flow in the non-ideal regime. Results reveal that the exploitation of pressure measurements only do not allow to infer the thermodynamic coefficients. Indeed, the material-dependent parameters remain highly uncertain.

7.1.7. Shape reconstruction of deposits inside a steam generator using eddy current measurements

H. Girardon, H. Haddar and L. Audibert

Non-destructive testing is an essential tool to assess the safety of the facilities within nuclear plants. In particular, conductive deposits on U-tubes in steam generators constitute a major danger as they may block the cooling loop. To detect these deposits, eddy-current probes are introduced inside the U-tubes to generate

currents and measuring back an impedance signal. Based on earlier work on this subject, we develop a shape optimization technique with regularized gradient descent to invert these measurements and recover the deposit shape. To deal with the unknown, and possibly complex, topological nature of the latter, we propose to model it using a level set function. The methodology is first validated on synthetic axisymmetric configurations and fast convergence in ensured by careful adaptation of the gradient steps and regularization parameters. We then consider a more realistic modeling that incorporates the support plate and the presence of imperfections on the tube interior section. We employ in particular an asymptotic model to take into account these imperfections and treat them as additional unknowns in our inverse problem. A multi-objective optimization strategy, based on the use of different operating frequencies, is then developed to solve this problem. Various numerical experimentations with synthetic data demonstrated the viability of our approach.

7.2. Invisiblity and transmission eigenvalues

7.2.1. 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 $\mathcal{PT}$-symmetric problems.

7.2.2. 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 $F^{\mathrm{a}} = F - \widetilde{F}$, where $\widetilde{F}$ is computed numerically, corresponding to well chosen artificial background and for which the associated TEs provide more accessible information on n.

7.2.3. 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.

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

F. Cakoni, H. Haddar and L. Audibert

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.

7.2.5. 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.

7.2.6. The spectral analysis of the interior transmission eigenvalue problem for Maxwell's equations

H. Haddar and S. Meng

we consider the transmission eigenvalue problem for Maxwell's equations corresponding to non-magnetic inhomogeneities with contrast in electric permittivity that has fixed sign (only) in a neighborhood of the boundary. Following the analysis made by Robbiano in the scalar case we study this problem in the framework of semiclassical analysis and relate the transmission eigenvalues to the spectrum of a Hilbert-Schmidt operator. Under the additional assumption that the contrast is constant in a neighborhood of the boundary, we prove that the set of transmission eigenvalues is discrete, infinite and without finite accumulation points. A notion of generalized eigenfunctions is introduced and a denseness result is obtained in an appropriate solution space.

7.2.7. Non reflection and perfect reflection via Fano resonance in waveguides

L. Chesnel, S.A. Nazarov

We investigate a time-harmonic wave problem in a waveguide. By means of asymptotic analysis techniques, we justify the so-called Fano resonance phenomenon. More precisely, we show that the scattering matrix considered as a function of a geometrical parameter ε and of the frequency λ is in general not continuous at a point $(\varepsilon, \lambda) = (0, \lambda^0)$ where trapped modes exist. In particular, we prove that for a given $\varepsilon \neq 0$ small, the scattering matrix exhibits a rapid change for frequencies varying in a neighbourhood of λ^0. We use this property to construct examples of waveguides such that the energy of an incident wave propagating through the structure is perfectly transmitted (non reflection) or perfectly reflected in monomode regime. We provide numerical results to illustrate our theorems.

7.2.8. From zero transmission to trapped modes in waveguides

L. Chesnel, V. Pagneux

We consider a time-harmonic scattering wave problem in a 2D waveguide at wavenumber k such that one mode is propagating in the far field. For a given k, playing with one scattering branch of finite length, we demonstrate how to construct geometries with zero transmission. The main novelty in this result is that the symmetry of the geometry is not needed: the proof relies on the unitary structure of the scattering matrix. Then, from a waveguide with zero transmission, we show how to build geometries supporting trapped modes associated with eigenvalues embedded in the continuous spectrum. For this second construction, using the augmented scattering matrix and its unitarity, we play both with the geometry and the wavenumber. The mathematical analysis is supplemented by numerical illustrations of the results.

7.3. Shape and topology optimization

7.3.1. Taking into account thermal residual stresses in topology optimization of structures built by additive manufacturing

G. Allaire and L. Jakabcin.

We introduce a model and several constraints for shape and topology optimization of structures, built by additive manufacturing techniques. The goal of these constraints is to take into account the thermal residual stresses or the thermal deformations, generated by processes like Selective Laser Melting, right from the beginning of the structural design optimization. In other words, the structure is optimized concurrently for its final use and for its behavior during the layer by layer production process. It is well known that metallic additive manufacturing generates very high temperatures and heat fluxes, which in turn yield thermal deformations that may prevent the coating of a new powder layer, or thermal residual stresses that may hinder the mechanical properties of the final design. Our proposed constraints are targeted to avoid these undesired effects. Shape derivatives are computed by an adjoint method and are incorporated into a level set numerical optimization algorithm. Several 2-d and 3-d numerical examples demonstrate the interest and effectiveness of our approach.

7.3.2. Topology optimization of modulated and oriented periodic microstructures by the homogenization method

G. Allaire, P. Geoffroy-Donders and O. Pantz

This work is concerned with the topology optimization of structures made of periodically perforated material, where the microscopic periodic cell can be macroscopically modulated and oriented. The main idea is to optimize the homogenized formulation of this problem, which is an easy task of parametric optimization, then to project the optimal microstructure at a desired lengthscale, which is a delicate issue, albeit computationally cheap. The main novelty of our work is, in a plane setting, the conformal treatment of the optimal orientation of the microstructure. In other words, although the periodicity cell has varying parameters and orientation throughout the computational domain, the angles between its members or bars are conserved. The main application of our work is the optimization of so-called lattice materials which are becoming increasingly popular in the context of additive manufacturing. Several numerical examples are presented for single and multiple loads problems, as well as for compliance or more general objective functions.

7.3.3. Shape optimization of a coupled thermal fluid-structure problem in a level set mesh evolution framework

G. Allaire, F. Feppon, F. Bordeu, J. Cortial and C. Dapogny

Hadamard's method of shape differentiation is applied to topology optimization of a weakly coupled three physics problem. The coupling is weak because the equations involved are solved consecutively, namely the steady state Navier-Stokes equations for the fluid domain, first, the convection diffusion equation for the whole domain, second, and the linear thermo-elasticity system in the solid domain, third. Shape sensitivities are derived in a fully Lagrangian setting which allows us to obtain shape derivatives of general objective functions. An emphasis is given on the derivation of the adjoint interface condition dual to the one of equality of the normal stresses at the fluid solid interface. The arguments allowing to obtain this surprising condition are specifically detailed on a simplified scalar problem. Numerical test cases are presented using a level set mesh evolution method. It is demonstrated how the implementation enables to treat a variety of shape optimization problems.

7.3.4. Optimizing supports for additive manufacturing

G. Allaire and B. Bogosel

In additive manufacturing process support structures are often required to ensure the quality of the final built part. In this article we present mathematical models and their numerical implementations in an optimization loop, which allow us to design optimal support structures. Our models are derived with the requirement that they should be as simple as possible, computationally cheap and yet based on a realistic physical modeling. Supports are optimized with respect to two different physical properties. First, they must support overhanging regions of the structure for improving the stiffness of the supported structure during the building process. Second, supports can help in channeling the heat flux produced by the source term (typically a laser beam) and thus improving the cooling down of the structure during the fabrication process. Of course, more involved constraints or manufacturability conditions could be taken into account, most notably removal of supports. Our work is just a first step, proposing a general framework for support optimization. Our optimization algorithm is based on the level set method and on the computation of shape derivatives by the Hadamard method. In a first approach, only the shape and topology of the supports are optimized, for a given and fixed structure. In second and more elaborated strategy, both the supports and the structure are optimized, which amounts to a specific multiphase optimization problem. Numerical examples are given in 2-d and 3-d.

7.3.5. Structural optimization under internal porosity constraints using topological derivatives

G. Allaire, J.Martinez-Frutos, C. Dapogny, F. Periago

Porosity is a well-known phenomenon occurring during various manufacturing processes (casting, welding, additive manufacturing) of solid structures, which undermines their reliability and mechanical performance. The main purpose of this article is to introduce a new constraint functional of the domain which controls the negative impact of porosity on elastic structures in the framework of shape and topology optimization. The main ingredient of our modelling is the notion of topological derivative, which is used in a slightly unusual way: instead of being an indicator of where to nucleate holes in the course of the optimization process, it is a component of a new constraint functional which assesses the influence of pores on the mechanical performance of structures. The shape derivative of this constraint is calculated and incorporated into a level set based shape optimization algorithm. Our approach is illustrated by several two- and three-dimensional numerical experiments of topology optimization problems constrained by a control on the porosity effect.

7.4. Analysis of some wave problems

7.4.1. On well-posedness of time-harmonic problems in an unbounded strip for a thin plate model

L. Bourgeois, L. Chesnel, S. Fliss

We study the propagation of elastic waves in the time-harmonic regime in a waveguide which is unbounded in one direction and bounded in the two other (transverse) directions. We assume that the waveguide is thin in one of these transverse directions, which leads us to consider a Kirchhoff-Love plate model in a locally perturbed 2D strip. For time harmonic scattering problems in unbounded domains, well-posedness does not hold in a classical setting and it is necessary to pre- scribe the behaviour of the solution at infinity. This is challenging for the model that we consider and constitutes our main contribution. Two types of boundary conditions are considered: either the strip is simply supported or the strip is clamped. The two boundary conditions are treated with two different methods. For the simply supported problem, the analysis is based on a result of Hilbert basis in the transverse section. For the clamped problem, this property does not hold. Instead we adopt the Kondratiev's approach, based on the use of the Fourier transform in the unbounded direction, together with techniques of weighted Sobolev spaces with detached asymptotics. After introducing radiation conditions, the corresponding scattering problems are shown to be well-posed in the Fredholm sense. We also show that the solutions are the physical (outgoing) solutions in the sense of the limiting absorption principle.

7.4.2. Crime Pays: Homogenized Wave Equations for Long Times

G. Allaire, A. Lamacz and J. Rauch

This work examines the accuracy for large times of asymptotic expansions from periodic homogenization of wave equations. As usual, ϵ denotes the small period of the coefficients in the wave equation. We first prove that the standard two scale asymptotic expansion provides an accurate approximation of the exact solution for times t of order $\epsilon^{-2+\delta}$ for any $\delta > 0$. Second, for longer times, we show that a different algorithm, that is called criminal because it mixes different powers of ϵ, yields an approximation of the exact solution with error $O(\epsilon^N)$ for times ϵ^{-N} with N as large as one likes. The criminal algorithm involves high order homogenized equations that, in the context of the wave equation, were first proposed by Santosa and Symes and analyzed by Lamacz. The high order homogenized equations yield dispersive corrections for moderate wave numbers. We give a systematic analysis for all time scales and all high order corrective terms.

7.5. Diffusion MRI

7.5.1. A partition of unity finite element method for computational diffusion MRI

D. V. Nguyen, J. Jansson, J. Hoffman and J.-R. Li.

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 inside 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 entire 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. In this paper, 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 are based on the partition of unity concept which allows for a discontinuous solution across interfaces conforming with the mesh with weak enforcement of real (in the case of interior interfaces) and artificial (in the case of exterior boundaries) permeability conditions as well as an operator splitting for the exterior boundary conditions. The method is straightforward to implement and it is available in FEniCS for moderate-scale simulations and in FEniCS-HPC for large-scale simulations. The order of accuracy of the resulting method is validated in numerical tests and a good scalability is shown for the parallel implementation. We show that the simulated dMRI signals offer good approximations to reference signals in cases where the latter are available and we performed simulations for a realistic model of a neuron to show that the method can be used for complex geometries.

7.5.2. Diffusion MRI simulation in thin-layer and thin-tube media using a discretization on manifolds

D. V. Nguyen, J. Jansson, H. T. A. Tran, J. Hoffman and J.-R. Li.

The Bloch-Torrey partial differential equation describes the evolution of the transverse magnetization of the imaged sample under the influence of diffusion-encoding magnetic field gradients inside the MRI scanner. The integral of the magnetization inside a voxel gives the simulated diffusion MRI signal. This paper proposes a finite element discretization on manifolds in order to simulate the diffusion MRI signal in domains that have a thin layer or a thin tube geometrical structure. Suppose that the three-dimensional domain has a thin layer structure: points in the domain can be obtained by starting on the two-dimensional manifold and moving along a depth (thickness) function. For this type of domains, we propose a finite element discretization formulated on a surface triangulation of the manifold. The variable thickness of the domain is included in the weak formulation on the surface triangular elements. A simple modification extends the approach to ‘thin tube’ domains where a manifold in one dimension and a two-dimensional variable cross-section describe the points

in the domain. We conducted a numerical study of the proposed approach by simulating the diffusion MRI signals from the extracellular space (a thin layer medium) and from neurons (a thin tube medium), comparing the results with the reference signals obtained using a standard three-dimensional finite element discretization. We show good agreement between the simulated signals using our proposed method and the reference signals. The approximation becomes better as the diffusion time increases. The method helps to significantly reduce the required simulation time, computational memory, and difficulties associated with mesh generation, thus opening the possibilities to simulating complicated structures at low cost for a better understanding of diffusion MRI in the brain.

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

K. V. Nguyen, D. Le Bihana, L. Ciobanua and J.-R. Li

The nerve cells of the *Aplysia* are much larger than mammalian neurons. Using the *Aplysia* ganglia to study the relationship between the cellular structure and the diffusion MRI signal can 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 and observed at low b-values, the dMRI signal is mono-exponential and can be accurately represented by the parameter ADC (Apparent Diffusion Coefficient).

We performed numerical simulations of water diffusion for three types of cells in the abdominal ganglia: the large cell neurons, the bag cells, and the nerve cells. For the bag cells and nerves cells, we created spherical and cylindrical geometrical configurations that are consistent with known information about the cellular structures from the literature. We used the simulation results to obtain information about the intrinsic diffusion coefficient in these cells.

For the large cell neurons, we created geometrical configurations by segmenting high resolution T_2-weighted (T_2w) images to obtain the cell outline and then incorporated a manually generated nucleus. We used numerical simulations to validate the claim that water diffusion in the large cell neurons is in the short diffusion time regime for our experimental diffusion times.

Then, using the analytical short time approximation (STA) formula for the ADC, we showed that in order to explain the experimentally observed behavior in the large cell neurons, it is necessary to consider the nucleus and the cytoplasm as two separate diffusion compartments. By using a two compartment STA model, we were able to illustrate the effect of the highly irregular shape of the cell nucleus on the ADC.

7.5.4. The derivation of homogenized diffusion kurtosis models for diffusion MRI

H. Haddar, M. Kchaou and M. Moakher

We use homogenization theory to establish a new macroscopic model for the complex transverse water proton magnetization in a voxel due to diffusion-encoding magnetic field gradient pulses in the case of biological tissue with impermeable membranes. In this model, new higher-order diffusion tensors emerge and offer more information about the structure of the biological tissues. We explicitly solve the macroscopic model to obtain an ordinary differential equation for the diffusion MRI signal that has similar structure as diffusional kurtosis imaging models. We finally present some validating numerical results on synthetic examples showing the accuracy of the model with respect to signals obtained by solving the Bloch-Torrey equation.

7.5.5. On-going collaborative projects on DMRI

J.R. Li, H. Haddar and I. Mekkaoui

- We performed simulations for a collaborative project with Demian Wassermann of the Parietal team on distinguishing between Spindle and pyramidal neurons with Multi-shell Diffusion MRI.
- We continue in the simulation and modeling of heart diffusion MRI with the post-doc 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.

7.6. Mathematical tools for Psychology

J. R. Li and J. Hao

This is the start of a collaborative effort between the Defi team and Dr. Hassan Rahioui 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.

  Result: unfortunately Jingjing Hao will not be able to continue with this PhD project as of Jan 2019. We will modify the project in consultation with Dr. Rahioui and continue it in another format.

7.7. Shape optimization under uncertainties

7.7.1. Surrogate-Assisted Bounding-Box Approach Applied to Constrained Multi-Objective Optimisation Under Uncertainty

P.M. Congedo, M. Rivier

This work is devoted to tackling constrained multi-objective optimisation under uncertainty problems. In particular, the SABBa (Surrogate-Assisted Bounding-Box approach) framework is applied and extended to handle both robust and reliability-based constrained optimisation problems. This approach aims at efficiently dealing with uncertainty-based optimisation problems, with approximated robustness and reliability measures. A Bounding-Box (or conservative box) is defined as a multi-dimensional product of intervals centred on approximated objectives and constraints and containing the underlying true values. In SABBa, this approach is supplemented with a Surrogate-Assisting strategy, which is very effective to reduce the overall computational cost, notably during the last iterations of the optimisation. The efficiency of the method is further increased using the concept of Pareto Optimal Probability (POP) computed for each box, and proposing some estimations for conservative error computation and box refinement using a Gaussian Process (GP).

7.7.2. A quantile-based optimization under uncertainty of an ORC turbine cascade

P.M. Congedo, N. Razaaly

This study presents an original and fast robust shape optimization approach to overcome the limitation of a deterministic optimization that neglects operating conditions variability, applied on a typical 2D ORC turbine cascade (Biere). Flow around the blade is solved by means of inviscid simulation using the open-source SU2 code, considering Non-Ideal gas effects modeled through the use of the Peng-Robinson-Stryjek-Vera equation of state, from which a Quantity of Interest (QoI) is recovered. We propose here a mono-objective formulation consisting in minimizing the α-quantile of the QoI under a constraint, at a low computational cost. This is performed by using an efficient robust optimization approach, coupling a state-of- the-art quantile estimation and a classical bayesian optimization method. First, the advantages of a quantile-based formulations are illustrated with respect to a classical mean-based robust optimization. Secondly, we demonstrate the effectiveness of applying this robust optimization framework with a low-fidelity inviscid solver by comparing the resulting optimal design with the ones obtained with a deterministic optimization using a high-fidelity turbulent solver.

7.8. Uncertainty Quantification methods for uncertainty propagation

7.8.1. Kriging-sparse Polynomial Dimensional Decomposition surrogate model with adaptive refinement

P.M. Congedo, A. Cortesi, G. El Jannoun

In this work, an algorithm for the construction of a low-cost and accurate metamodel is proposed, having in mind redcomputationally expensive applications. It has two main features. First, Universal Kriging is coupled 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 a Universal Kriging surrogate model. Secondly, a numerical method, derived from anisotropic mesh adaptation, is formulated in order to adaptively insert a fixed number of new training points to an existing Design of Experiments. The convergence of the proposed algorithm is analyzed and assessed on different test functions with an increasing size of the input space. Finally, the algorithm is used to propagate uncertainties in two high-dimensional real problems related to the atmospheric reentry.

7.8.2. Novel algorithm using Active Metamodel Learning and Importance Sampling: Application to multiple failure regions of low probability

P.M. Congedo, N. Razaaly

Calculation of tail probabilities is of fundamental importance in several domains, such as in risk assessment. One major challenge consists in the computation of low-failure probability in cases characterized by multiple-failure regions, especially when an unbiased estimation of the error is required. Methods developed in literature rely mostly on the construction of an adaptive surrogate, tackling some problems such as the metamodel building criterion and the global computational cost, at the price of a generally biased estimation of the failure probability. In this work, we propose a novel algorithm suitable for low-failure probability and multiple-failure regions, permitting to both building an accurate metamodel and to provide a statistically consistent error. Indeed, an importance sampling technique is used, which is quasi-optimal since permits, by exploiting the knowledge of the metamodel, to provide two unbiased estimators of the failure probability. Additionally, a gaussian mixture-based importance sampling technique is proposed, permitting to drastically reduce the computational cost when estimating some reference values, or the failure probability directly from the metamodel. Several numerical examples are carried out, showing the very good performances of the proposed method with respect to the state-of-the-art in terms of accuracy and computational cost. A physical test-case, focused on the numerical simulation of non-ideal gas turbine cascades, is also investigated to illustrate the capabilities of the method on an industrial case.

7.8.3. Uncertainty propagation framework for systems of codes

P.M. Congedo, F. Sanson, O. Le Maitre

The simulation of complex multi-physics phenomena often requires the use of coupled solvers, modelling different physics (fluids, structures, chemistry, etc) with largely differing computational complexities. We call Systems of Solvers (SoS) a set of interdependent solvers where the output of an upstream solver can be the input of a downstream solvers. In this work we restrict ourselves to weakly coupled problems. A system of solvers typically encapsulate a large number of uncertain input parameters, challenging classical Uncertainty Quantification (UQ) methods such as spectral expansions and Gaussian process models which are affected by the curse of dimensionality. In this work, we develop an original mathematical framework, based on Gaussian Processes (GP) to construct a global metamodel 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 of the SoS. These local GP models are built adaptively to satisfy criteria based on the global output error estimation, which can be decomposed (following an ANOVA-like decomposition) into contributions from individual GP models. This decomposition enables one to select the local GP models that need be refined to efficiently reduce the global error using computer experiment design methods or Bayesian optimization. This framework is then applied to a space object reentry problem.

7.9. Application of Uncertainty Quantification studies to fluid-dynamics problems

7.9.1. Validation of the Non-Ideal Compressible-Fluid Dynamics solver from the open-source SU2 suite

P.M. Congedo, G. Gori, A. Guardone, M. Zocca

The first-ever experimental validation of a flow simulation software for Non-Ideal Compressible-Fluid Dynamics (NICFD) flows is presented. Numerical results from the open-source suite SU2 are compared against pressure and Mach number measurements of supersonic flows of siloxane fluid MDM (Octamethyltrisiloxane, $C_8H_{24}O_2Si_3$) at conditions in the close proximity of the liquid-vapour saturation curve. The test set is representative of typical operating conditions of Organic Rankine Cycle systems and it includes expanding flows through a converging-diverging nozzle in mildly-to-highly non-ideal conditions. The validation process takes advantage of an Uncertainty Quantification analysis, to estimate the variability of the numerical solution with respect to the physical uncertainties and to provide a robust assessment of the SU2 capabilities. All considered flows are well represented by the numerical solutions and therefore the reliability of the numerical implementation and the predictiveness of the NICFD solver are confirmed.

7.9.2. Impact of geometric, operational, and model uncertainties on the non-ideal flow through a supersonic ORC turbine cascade

P.M. Congedo, N. Razaaly, G. Persico

Typical energy sources for Organic Rankine Cycle (ORC) power systems feature variable heat load and turbine inlet/outlet thermodynamic conditions. The use of organic compounds with heavy molecular weight introduces uncertainties in the fluid thermodynamic modeling. In addition, the peculiarities of organic fluids typically lead to supersonic turbine configurations featuring supersonic flows and shocks, which grow in relevance in the aforementioned off-design conditions; these features also depend strongly on the local blade shape, which can be influenced by the geometric tolerances of the blade manufacturing. This study presents an Uncertainty Quantification (UQ) analysis on a typical supersonic nozzle cascade for ORC applications, by considering a two-dimensional high-fidelity turbulent Computational Fluid Dynamic (CFD) model. Kriging-based techniques are used in order to take into account at a low computational cost, the combined effect of uncertainties associated to operating conditions, fluid parameters, and geometric tolerances. The geometric variability is described by a finite Karhunen-Loeve expansion representing a non-stationary Gaussian random field, entirely defined by a null mean and its autocorrelation function. Several results are illustrated about the ANOVA decomposition of several quantities of interest for different operating conditions, showing the importance of geometric uncertainties on the turbine performances.

7.9.3. Efficient surrogate based human risk estimation of a space object reentry

P.M. Congedo, F. Sanson, O. Le Maitre, J.-M. Bouilly, C. Bertorello

The prediction of risk associated with the reentry of a man made space object is critical but subject to input parameter uncertainties. To compute the risk one needs to determine whether the object survives to reentry and if it does where it falls on Earth. Expensive numerical models can be used to answer both questions but they can only be evaluated a limited number of times to propagate the uncertainties. In this work, we present an original approach to construct an accurate surrogate model of the numerical models using a limited number of solver evaluations. Using Gaussian Processes, the constructed surrogate model is able two answer both questions (survivability and impact location) in order to provide an accurate description of the risk. The surrogate model can achieve high level of accuracy in terms of risk estimation using dedicated active learning strategies. The efficiency of the method is illustrated on analytical test cases and an actual space object reentry case.

ECUADOR Project-Team

6. New Results

6.1. Towards Algorithmic Differentiation of C++

Participants: Laurent Hascoët, Valérie Pascual, Frederic Cazals [ABS team, Inria Sophia-Antipolis].

We made progress towards the extension of Tapenade for C++. Last year, an external parser for C++ was built on top of Clang-LLVM https://clang.llvm.org/ and connected to the input formalism "IL" of Tapenade, but the internals of Tapenade were not able to handle the new constructs present in this input. This year, integration of C++ was pushed further by taking into account many of the new constructs (namespaces, classes, constructors and destructors) in the Internal Representation(IR) of Tapenade. Not surprisingly, this implied deep changes in several areas of Tapenade code. The IR of Tapenade now contains classes, constructors and destructors, and also has a faithful representation for namespaces. The textual nested structure and the control-flow parts of the IR are correct. The symbol tables and the representation for memory locations are still under development.

As a result, Tapenade is now able to input its first C++ files and is able to output them, but without transformation. Although not advertised nor documented, the functionality is present in the latest release 3.14. Data-Flow analysis and code transformation (e.g. AD) will not be possible until we have a correct IR about variables and their memory locations. This work is going on.

This work benefited from the expertise in C++ of Frederic Cazals (Inria ABS team). The ABS team provided a large test application code (SBL, https://sbl.inria.fr/) for Molecular Dynamics, which will be our first C++ target.

6.2. AD of mixed-language codes

Participants: Valérie Pascual, Laurent Hascoët.

Last year Tapenade was extended to differentiate codes that mix different languages, beginning with the tangent mode of AD. Our motivating application here is Calculix, a 3-D Structural Finite Element code that mixes Fortran and C. This year, we continued development towards Adjoint Differentiation. Although more complete testing is needed, we now have a first correct adjoint of Calculix.

Tapenade can now routinely differentiate Fortran+C codes, and accepts and takes advantage of the interoperability directives provided by the Fortran 2003 standard. It can handle not only procedure parameters correspondence, but also interoperability between C `struct` and Fortran `COMMON` blocks. Laurent Hascoët presented the advancement of this work at the ISMP 2018 congress in Bordeaux https://ismp2018.sciencesconf.org/.

C files (aka "translation units") and Fortran modules are two instances of the more general notion of "package" for which we are looking for a unified representation in Tapenade. It appears that this common representation could also handle C++ namespaces.

6.3. Differentiation of non-smooth programs

Participants: Laurent Hascoët, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)].

Algorithmic Differentiation can be used to derive tangent models that cope with a certain class of non-smoothness, through the use of the so-called Abs-Normal Form (ANF) [23]. These tangent models incorporate some knowledge of the nearby discontinuities of the derivatives. These models bring some additional power to processes that use tangent approximations, such as simulation, optimization, or solution of differential equations.

The mechanics to derive these special tangent models can be built as an extension of standard tangent linear Algorithmic Differentiation. This has been first demonstrated by the AD tool AdolC which, being based on Operator Overloading, is more flexible and seems a natural choice for implementation. Together with Krishna Narayanan, we recently tried a similar adaption on Source-Transformation AD tools. It appears that very little development is needed in the AD-tool. Specifically for Tapenade, it appears that no development at all is needed in the tool itself. Any end-user can already produce ANF tangent without needing any access to the tool source. All it requires is a customized derivative of the absolute-value function (ABS), which is currently less than 40 lines of code.

Building the ANF of a given program introduces one new variable per run-time execution of the ABS function. As the number of rows and columns of the constructed extended Jacobian both grow like the number of variables, it may become unreasonably large for large codes. To overcome this issue, we explore the possibility of finding at run-time the "important" ABS calls that deserve this treatment, and those that don't. We base this decision on a notion of distance to the kink induced by this ABS call as illustrated by Figure 2 . We presented these experiments at a Shonan meeting on this question (Shonan, Japan, June 25-29) and at a workshop of ISMP 2018 (Bordeaux, July 2-6)

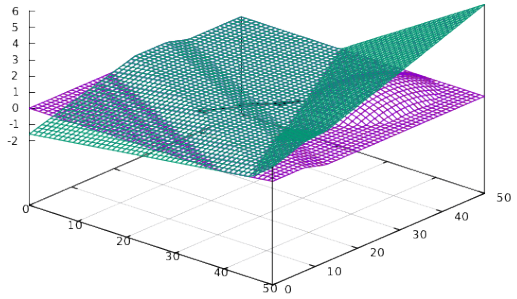


Figure 2. Abs-Normal Form of a non-smooth function: purple:original function, green ANF computed at (30,30). The ANF is linearized around the point of interest, and at the same time captures the non-smooth behavior. Notice the ANF divergence from the original function on the left, due to neglecting the leftmost kink which was decided "far" enough from the point of interest. The ANF divergence on the right is the natural effect of linearization

6.4. AD-adjoints and C dynamic memory management

Participants: Laurent Hascoët, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, 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 requires 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, trying to prove correctness of our current address conversion, we discovered some limitations that indeed made the proof impossible. To solve these issues, it seems necessary to assign at run-time a unique identifier to each chunk of memory used by the code, and to carry this identifier along with every pointer. This results in a code transformation which, although more complex than expected, can still be described by a small set of rewrite rules. Moreover, this alternative method should reduce the run-time overhead that we observed previously. Implementation and measurements are still under way. We presented this recent research in the form of a catalogue of alternatives for Data-Flow reversal of memory addresses, at the 21st EuroAD workshop (Jena, Germany, November 19-20).

6.5. Application to large industrial codes

Participants: Valérie Pascual, Laurent Hascoët, Bruno Maugars [ONERA], Sébastien Bourasseau [ONERA], Bérenger Berthoul [ONERA].

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

This year's main application is with ONERA on their ElsA CFD platform (Fortran 90). Both tangent and adjoint models of the kernel of ElsA were built successfully by Tapenade. It is worth noticing that this application was performed inside ONERA by ONERA engineers (Bruno Maugars, Sébastien Bourasseau, Bérenger Berthoul) with no need for installation of ElsA inside Inria. We take this as a sign of maturity of Tapenade. Apart from a few minor corrections, our contributon was essentially during development meetings, to point out some strategies and tool options to obtain efficient differentiated code. One emphasis was on adjoint of vectorized code, which was produced as vectorized code too by means of a seldom-used Tapenade option that stores intermediate values statically, i.e. not on a global stack. Sébastien Bourasseau presented the first results at the 21st EuroAD workshop (Jena, Germany, November 19-20), with convincing performance on industrial-size test cases. A joint article is in preparation.

6.6. Multirate methods

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

This study is performed in collaboration with IMAG-Montpellier. It addresses an important complexity issue in unsteady mesh adaptation and took place in the work done in the ANR Maidesc (ended 2017). 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 stretched since only very few cells are in the regions of small time-step constraint. 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. A novel analysis shows that the proposed multirate algorithm indeed solves the unsteady mesh adaptation barrier identified in previous works. This work is being published in a journal [13].

6.7. 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.

This year, two conference papers were written on the methods of the team, including new analyses in [11],[10], a work on correctors in CFD in an AIAA paper. A detailed study of adjoint-based mesh adaptation for Navier-Stokes flows has been completed and published in a journal [9].

Following participation of Gamma3 and Ecuador to the European project UMRIDA (ended 2017), we wrote chapters 20, 21, 45, and 48 of the book "Uncertainty Management for Robust Industrial Design in Aeronautics", edited by C. Hirsch et al. in the Springer series Notes on Numerical Fluid Mechanics and Multidisciplinary Design (2019).

6.8. 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.

This year, we have developed a new model relying on the hybridation of a DDES model based on a k-ϵ closure with our dynamic VMS model. This model shows improvement in most situations and in particular for laminar flows.

We have also addressed this year a challenging test case, the flow around tandem cylinders with a distance between the cylinders of 12 diameters. The accurate capture of the vortices traveling along this path of 12 diameters requires that the LES filter does not accumulate any dissipation along this trajectory. This is a noticeable property or our DVMS model. Further, the numerics need be as accurate as possible. We use a superconvergent approximation, up to fifth order accurate on Cartesian regions of the computational domain. This combination allowed for an accurate prediction of the drag of the second cylinder. This result has been presented at the workshop ETMM12 [12]

ELAN Team

6. New Results

6.1. 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 been published in Roy. Soc. Proc A [1] and physical aspects of this study have been communicated about in a mechanical congress [4].

6.2. Simulation of cloth contact with exact Coulomb friction

Participants: Florence Bertails-Descoubes, Laurence Boissieux.

In collaboration with Gilles Daviet (Weta Digital, New Zealand) and Rahul Narain's group (University of Minnesota and IIT Delhi), 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 an unprecedent level of realism compared to former methods, while maintaining similar computational timings. Our work has been published at ACM Transactions on Graphics (ACM SIGGRAPH 2018) [2].

6.3. Inverse design of thin elastic shells

Participants: Mickaël Ly, Florence Bertails-Descoubes, Laurence Boissieux.

In collaboration with Romain Casati (former PhD student of F. Bertails-Descoubes) and Mélina Skouras (EPI IMAGINE), we have proposed an inverse strategy for modeling thin elastic shells physically, just from the observation of their geometry. Our algorithm takes as input an arbitrary target mesh, and interprets this configuration automatically as a stable equilibrium of a shell simulator under gravity and frictional contact constraints with a given external object. Unknowns are the natural shape of the shell (i.e., its shape without external forces) and the frictional contact forces at play, while the material properties (mass density, stiffness, friction coefficients) can be freely chosen by the user. Such an inverse problem formulates as an ill-posed nonlinear system subject to conical constraints. To select and compute a plausible solution, our inverse solver proceeds in two steps. In a first step, contacts are reduced to frictionless bilateral constraints and a natural shape is retrieved using the adjoint method. The second step uses this result as an initial guess and adjusts each bilateral force so that it projects onto the admissible Coulomb friction cone, while preserving global equilibrium. To better guide minimization towards the target, these two steps are applied iteratively using a degressive regularization of the shell energy. We validate our approach on simulated examples with reference material parameters, and show that our method still converges well for material parameters lying within a

reasonable range around the reference, and even in the case of arbitrary meshes that are not issued from a simulation. We finally demonstrate practical inversion results on complex shell geometries freely modeled by an artist or automatically captured from real objects, such as posed garments or soft accessories. Our work has been published at ACM Transactions on Graphics (ACM SIGGRAPH Asia 2018) [3] and has been selected for a Press Release of the ACM.

GAMMA3 Project-Team

5. New Results

5.1. The meshing bible

Participants: Paul-Louis George [The Boss], Houman Borouchaki, Frédéric Alauzet, Patrick Laug, Adrien Loseille, Loïc Maréchal.

Un projet important, initié en 2017, et amené à se poursuivre l'an prochain, consiste à écrire noir sur blanc un livre (en plusieurs volumes) et la motivation de ce travail est détaillée dans ce qui suit.

Pourquoi ce livre, pourquoi 2 volumes, pourquoi pas 3 volumes?

Notre dernier livre (généraliste) sur le maillage date de 2000 avec une mise à jour en 2008. Un collègue a commis un nouveau livre en 2015, très bien écrit mais assez classique dans son contenu, loin de préoccupations industrielles et (!) contenant quelques énormités (pas assez d'experience sur de vrais problèmes).

Ajoutons ma facilite (c'est P.L. G. qui parle) à écrire (bien ou mal, là n'est pas la question, il me suffit en effet de taper sur quelques touches d'un clavier), le désir de mon (premier) co-auteur de marquer le coup dans le domaine et la volonté (à leur corps defendant) des autres co-auteurs de participer à cette aventure. Le tout couplé avec les récents progrès dans le domaine (pensons aux éléments courbes et aux méthodes d'ordre élevé mais aussi à ce que peut être le HPC dans le domaine), tous les ingrédients sont là, on y va.

Le premier jet (un seul volume) se montre impossible à réaliser, il faudrait au minimum 800 pages, donc deux volumes a minima. Les deux volumes finis, ne reste il pas la place pour un troisième volume. Constatant avec effroi que nos étudiants (mais pas seulement) maitrisent bien force concepts mais sont incapables de voir, en pratique, comment les mettre en musique, le troisième volume est apparu comme une évidence (et on sera, au total, autour de 1000 pages).

A qui s'adresse ces volumes, bonne question. Ce n'est pas précisément de la littérature de gare mais nous nous sommes efforcé de prendre le malheureux lecteur par la main pour l'amener progressivement vers des concepts (très) avancés. Ainsi, le livre est très verbose et, en aucun cas, n'est un étalage savant de théorèmes et autres propositions, ce qui n'empêche pas de dire les choses. Par ailleurs, nous avons délibérément mis une part de subjectivité dans le propos pour suggérer (cela pouvant être contredit) que telle ou telle méthode n'avait pas notre faveur. A titre personnel, je pense que, bien que rares dans les livres, ces opinions ne peuvent qu'aider le lecteur a se former sa propre idée sur tel ou tel point.

Les livres sont publiés chez ISTE et écrits en français, eh oui, mais une traduction en anglais est avalable chez Wiley. La présence de la langue française dans la littérature scientifique me semble importante (et rejoint la politique de mon (notre) éditeur). Pour conclure, c'est plutôt satisfaisant de penser que ces livres (peut être destinés à faire référence sur le sujet) sont issus de l'Inria dans le neuf un.

5.2. Realistic modeling of fractured geologic media

Participants: Patrick Laug [correspondant], Géraldine Pichot.

This study started in 2016, in collaboration with the 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. Significant progress has been made during this year 2018, as we are now able to make geometric models and numerical simulations with more than 1 million fractures, 2 million intersections, and 18 million triangles, in about one hour on a laptop [7], [8], [19], [20], [21].

5.3. High order geometric modeling

Participants: Patrick Laug [correspondant], Houman Borouchaki.

In the area of geometric modeling, major challenges are linked to the efficient **visualization** of CAD surfaces and to the generation of **meshes** adapted to numerical simulation. In this context, the elaboration and implementation of a **discrete geometric model** provides a simple and universal representation model, without the need for CAD. A first study has been carried out for a model of degree 1 (one) defined by a "triangulation" composed of quadrilaterals and triangles. The advantage of this model of degree 1 lies in its geometric simplicity. However, in the case of complex surfaces, it may require a very large number of elements, and besides it is not sufficiently rich to give certain essential characteristics like geometric curvatures. The main goal of this project is to extend this discrete model of degree 1 to **higher degrees**. These studies are conducted by "MODIS", an Associate Team comprising members of research teams at Inria, UTT (France) and Polytechnique Montreal (Canada) from 2017 to 2019. This year (2018) has been mostly devoted to the software implementation of all the theoretical bases obtained last year. In particular, chapters 6 and 11 of a recent book [22] give data structures where a local numbering is recursively defined for any order of the elements.

5.4. Rendu pixel-exact de solutions d'ordre élevé

Participants: Adrien Loseille [correspondant], Rémi Feuillet.

Avec le développement des méthodes d'ordre élevé, il apparaît également important de visualiser de manière fidèle à la fois le maillage et la solution associée. L'objet de cette thématique de recherche est de mettre à profit les fonctionnalités de programmation du pipeline graphique de la bibliothèque graphique OpenGL 4.0 afin de mettre en place des techniques de rendu de solutions d'ordre élevé quasiment exactes au pixel près ainsi que des techniques rapides de visualisation d'éléments d'ordre élevé. Les premiers résultats sont très satisfaisants avec un rendu de solutions d'ordre élevé allant de l'ordre 1 à 5 et ce exact au pixel près si ces dernières sont représentées sur des maillages de degré 1. Au niveau de la représentation des éléments d'ordre élevé, la visualisation est possible jusqu'à l'ordre 4 avec visualisation d'une solution dessus. Cette dernière sera d'autant plus représentée au pixel près que la représentation de la géométrie courbe (pour des degrés plus grands que 1) sera exacte. Ce travail a fait en 2018 l'objet de deux exposés à des conférences, dont une publication [13] dans les *proceedings*: *AIAA Scitech* et *WCCM*. Les prochaines étapes vont se concentrer sur la représentation de solutions et d'éléments d'ordre élevés à travers un plan de coupe, à la représentation des iso-surfaces et enfin à l'optimisation de ce code.

5.5. Génération de maillages d'ordre élevé

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

En calcul scientifique, l'utilisation de solveurs d'ordre élevé (supérieur à deux) se fait croissante. Or ces solveurs ne sont fonctionnels que lorsqu'ils sont couplés avec des maillages d'ordre élevé, nécessaires pour une représentation d'ordre élevé de la géométrie. L'idée de cette thématique de recherche est de s'intéresser à la génération et à l'*amélioration* par modification locale de tels maillages. Dans cette optique, un générateur de maillages courbe en partant de maillages droit a été développé. Ensuite, une étude importante a été consacrée à la généralisation au degré 2 des opérateurs locaux classiques d'optimisation de maillage, à savoir la bascule d'arête/face (*swap*) et le bougé de point (*smoothing*). La généralisation de tels outils a permis d'une part de rendre la génération de maillages courbe plus robuste et d'autre part rendu possibles au degré 2 les techniques de maillage mobile avec changement local de connectivité. Ce travail a fait l'objet en 2018 de deux exposés sans *proceedings* à *ECCM-ECFD* et *ICOSAHOM* et de 2 exposés avec *peer-reviewed proceedings* à *AIAA Aviation* et à l'*International Meshing Roundtable* [9], [10]. La suite de ce travail va être de générer des maillages de couche limites directement courbes (en utilisant la technique de maillage courbe mobile) puis de se consacrer à la généralisation de ce travail à des ordres plus grands. Il sera aussi apporté un soin particulier à la génération de maillages de surface courbe à partir de modèles de CAO.

5.6. Adaptation de maillages pour des écoulements visqueux en turbomachine et aéro-externe

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

5.6.1. Calcul

Les principes d'une adaptation pour les écoulements Navier-Stokes turbulents ont été validés 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, 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 en aval. Des conditions limites bien précises ont donc été développées afin de traiter correctement ces effets.

5.6.2. Adaptation

Pour l'adaptation de maillages deux particularités doivent ètre traitées ici, la périodicité du maillage et la couche limite turbulente. En toute dimemsion, la couche limite a donc été traitée par des techniques d'adaptation. Le maillage est adapté dans le volume en utilisant la Hessienne du Mach de l'écoulement comme senseur. La périodicité est traitée en utilisant un noyau non-manifold de logiciel de remaillage `Feflo.a`.

Ces développements ont été présentés dans plusieurs conférences internationales et sont détaillés dans la thèse de Loïc Frazza [1], et dans le cadre d'une collaboration avec Safran Tech.

5.7. 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.

5.8. Adaptive boundary layer mesh generation

Participants: Adrien Loseille [correspondant], Victorien Menier.

Si des méthodes traditionnelles de couches limites sont désormais matures, elles sont souvent incompatibles dans un contexte adaptatif où les tailles varient dans la couche limite. On a développé dans ce cadre une méthode d'adaptation de la couche limite à la fois dans la direction normale et dans le plan tangent basée sur un couplage entre un opérateur de cavité contraint et une adaptation de surface interne.

5.9. Améliorations des schémas pour les simulation RANS

Participants: Loïc Frazza, Frédéric Alauzet [correspondant].

Grâce à une implémentation adéquate de schémas numériques modernes, nous avons montré qu'il est possible de réaliser des simulations RANS sur des maillages tétraédriques non structurés. Nous avons ainsi pu réaliser des calculs sur des maillages adaptés pour différentes applications industrielles complexes. A cette fin, nous avons réalisé l'analyse mathématiques nécessaire au développement des senseurs d'erreurs turbulents efficaces et précis. Nous avons également été amenés à étendre la résolution des variables adjointes aux modèles RANS. En comparant les performances de cette stratégie d'adaptation, nous avons pu montrer la supériorité des résultats obtenus en comparaison des méthodes hessiennes et traditionnelles sur différentes applications. Tous ces développements ont été validés dans le solveur `Wolf`, présentés et publiés dans [12], [6], [15] et ont été développés dans le cadre des collaborations avec Boeing et Safran Tech.

5.10. Deterministic smoothing parallelization

Participants: Lucille-Marie Tenkès, Frédéric Alauzet [correspondant].

On élabore des solutions algorithmiques pour paralléliser un opérateur géométrique d'optimisation de maillage, le bougé de points : une solution non-dynamique et une solution dynamique.

Le but est de paralléliser les méthodes de bougé de points de manière déterministe. En effet, avec les algorithmes actuels, le résultat de l'optimisation dépend de l'ordre dans lequel les points sont traités, qui n'est pas prévisible en parallélisation multi-thread asynchrone. Cela devient problématique lorsqu'on insère cette étape dans un processus global. S'il survient une erreur, on ne pourra pas reproduire les cas invalides pour apporter des corrections. Une première idée a été de rendre les calculs d'optimisation déterministes en implémentant une méthode non dynamique, qui prend comme référence pour le calcul des positions optimales la configuration initiale et non la configuration en cours d'optimisation. Une relaxation est effectuée une fois toutes les positions optimales calculées, et elle est globale. Cela permet d'avoir un bougé de points vraiment indépendant de l'ordre dans lequel les points sont traités. Cette méthode est bien déterministe, mais l'algorithme est moins efficace et plus lent que les méthodes de bougé de points dynamiques. L'alternative dynamique consiste à agir directement sur la parallélisation, en regroupant les points de manière à ne pas laisser les calculs interférer. L'idée est de créer une partition des nœuds en mettant dans une même classe ceux qui ne sont pas reliés entre eux par une arête. Ainsi, si l'un d'entre eux bouge lors du processus d'optimisation, il n'impactera pas ceux de sa classe. Cela revient donc à colorier ces sommets, de sorte que deux nœuds reliés par une arête n'aient pas la même couleur. L'algorithme choisi effectue un coloriage de proche en proche (approche frontale). La couleur 1 est attribuée au premier sommet, les points de sa boule sont coloriés par élimination, et ainsi de suite. Ces algorithmes ont été testés sur des maillages 2D et 3D pour caractériser leurs performances. Il en ressort que la méthode dynamique est assez efficace et rapide pour être appliquée à des maillages 3D de grande taille. De plus, l'étape de partition a été elle-même parallélisée et optimisée.

5.11. Opérateurs d'optimisation de maillage alignés et maillages quad-dominants

Participants: Lucille-Marie Tenkès, Frédéric Alauzet [correspondant].

On se base ici sur les méthodes de maillage par alignement des éléments sur la métrique. C'est-à-dire que les éléments du maillage, en plus de présenter une taille adaptée à la solution, suivent une direction prescrite. Une des difficultés ressortant de cette méthode est l'optimisation par bougé de points, car cela rompt l'alignement. On veut donc ici mettre en place une technique de bougé de points permettant de corriger, sans en détruire la structure, un maillage généré par alignement sur la métrique. Les modifications apportées à l'optimiseur sont un opérateur de réduction d'arête, une procédure d'appariement en quadrilatères, et un opérateur de bougé de points utilisant ces quadrilatères.

5.12. Multi-physic mesh adaptation

Participants: Frédéric Alauzet [correspondant], Rémi Feuillet, Julien Vanharen.

A new strategy [18] for mesh adaptation dealing with Fluid-Structure Interaction (FSI) problems is presented using a partitioned approach. The Euler equations are solved by an edge-based Finite Volume solver whereas the linear elasticity equations are solved by the Finite Element Method using the Lagrange P1 elements. The coupling between both codes is realized by imposing boundary conditions. Small displacements of the structure are assumed and so the mesh is not deformed. The computation of a well-documented FSI test case is finally carried out to perform validation of this new strategy. The capability of treating three-dimensional complex cases is also demonstrated.

MATHERIALS Project-Team

6. New Results

6.1. Electronic structure calculations

Participants: Robert Benda, 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.

6.1.1. Mathematical analysis

The members of the team have continued their systematic study of the properties of materials in the reduced Hartree-Fock approximation, a model striking a good balance between mathematical tractability and the ability to reproduce qualitatively complex effects.

E. Cancès and G. Stoltz have studied with L. Cao models for certain extended defects in materials [37]. These extended defects typically correspond to taking out a slab of finite width in the three-dimensional homogeneous electron gas. The work is performed in the framework of the reduced Hartree-Fock model with either Yukawa or Coulomb interactions, using techniques previously developed to study local perturbations of the free-electron gas. It is shown that the model admits minimizers, and that Yukawa ground state energies and density matrices converge to ground state Coulomb energies and density matrices as the Yukawa parameter tends to zero. These minimizers are unique for Yukawa interactions, and are characterized by a self-consistent equation. Numerical simulations show evidence of Friedel oscillations in the total electronic density.

A. Levitt has examined the phenomenon of screening in materials. In [54] he has studied the effect of adding a small charge to a periodic system modeled by the reduced Hartree-Fock at finite temperature. He has showed that the reaction potential created by the rearrangement of the electrons counteracts exactly the free charge, so that the effective interaction in such systems is short-range. The proof proceeds by studying the properties of the linear response operator, which also sheds some light on the charge-sloshing instability seen in numerical methods to solve the self-consistent equations.

6.1.2. Numerical analysis

E. Cancès has pursued his long-term collaboration with Y. Maday (Sorbonne Université) on the numerical analysis of linear and nonlinear eigenvalue problems. Together with G. Dusson (Warwick, United Kingdom), B. Stamm (Aachen, Germany), and M. Vohralík (Inria SERENA), they have designed *a posteriori* error estimates for conforming numerical approximations of the Laplace eigenvalue problem with homogeneous Dirichlet boundary conditions. In [38], they prove *a priori* error estimates for the perturbation-based post-processing of the plane-wave approximation of Schrödinger equations introduced and tested numerically in previous works. They consider a Schrödinger operator $H = -\frac{1}{2}\Delta + V$ on $L^2(\Omega)$, where Ω is a cubic box with periodic boundary conditions. The quantities of interest are, on the one hand, the ground-state energy defined as the sum of the lowest N eigenvalues of H , and, on the other hand, the ground-state density matrix, that is the spectral projector on the vector space spanned by the associated eigenvectors. Such a problem is central in first-principle molecular simulation, since it corresponds to the so-called linear subproblem in Kohn-Sham density functional theory (DFT). Interpreting the exact eigenpairs of H as perturbations of the numerical eigenpairs obtained by a variational approximation in a plane-wave (i.e. Fourier) basis, they compute first-order corrections for the eigenfunctions, which are turned into corrections on the ground-state density matrix. This allows them to increase the accuracy of both the ground-state energy and the ground-state density matrix at a low computational extra-cost. Indeed, the computation of the corrections only requires the computation of the residual of the solution in a larger plane-wave basis and $2N$ Fast Fourier Transforms.

Implicit solvation models aim at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous medium accounting for long-range electrostatics. E. Cancès, Y. Maday (Sorbonne Université), and B. Stamm (Aachen, Germany) have introduced a few years ago a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. In collaboration with F. Lipparini and B. Mennucci (Chemistry, Pisa, Italy) and J.-P. Piquemal (Sorbonne Université), they have implemented this algorithm in widely used computational software products (Gaussian and Tinker). Together with L. Lagardère (Sorbonne Université) and G. Scalmani (Gaussian Inc., USA), they illustrate in [29] the domain decomposition COSMO (ddCOSMO) implementation and how to couple it with an existing classical or quantum mechanical (QM) codes. They review in detail what input needs to be provided to ddCOSMO and how to assemble it, describe how the ddCOSMO equations are solved and how to process the results in order to assemble the required quantities, such as Fock matrix contributions for the QM case, or forces for the classical one. Throughout the paper, they make explicit references to the ddCOSMO module, which is an open source, Fortran 90 implementation of ddCOSMO that can be downloaded and distributed under the LGPL license.

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 in [39] the speed of convergence for a number of schemes in the metallic case, and have 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. With A. Damle (Cornell, USA) and L. Lin (Berkeley, USA), they have proposed an efficient numerical method for the computation of maximally-localized Wannier functions in metals, and have showed on the example of the free electron gas that they are not in general exponentially localized [42]. 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 [45].

6.2. Computational Statistical Physics

Participants: Grégoire Ferré, Florent Hédin, Frédéric Legoll, Tony Lelièvre, 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, using concepts of statistical physics (thermodynamic ensembles and molecular dynamics). The contributions of the team can be divided into four main topics: (i) the development of methods for sampling the configuration space; (ii) the numerical analysis of such methods; (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.

6.2.1. Sampling of the configuration space: new algorithms and applications

New numerical methods in order to sample probability measures on the configuration space have been developed: either measures supported on submanifolds, or stationary states of stochastic dynamics. First, in [51], T. Lelièvre and G. Stoltz, together with M. Rousset (Inria Rennes, France) have studied how to sample probability measures supported on submanifolds, by adding an extra momentum variable to the state of the system, and discretizing the associated Hamiltonian dynamics with some stochastic perturbation in the extra variable. In order to avoid biases in the invariant probability measures sampled by discretizations of these stochastically perturbed Hamiltonian dynamics, a Metropolis rejection procedure can be considered. The so-obtained scheme belongs to the class of generalized Hybrid Monte Carlo (GHMC) algorithms. However, the usual method has to be generalized using a procedure suggested by Goodman, Holmes-Cerfon and Zappa for Metropolis random walks on submanifolds, where a reverse projection check is performed to enforce the reversibility of the algorithm for large timesteps and hence avoid biases in the invariant measure. A full mathematical analysis of such procedures is provided, as well as numerical experiments demonstrating the

importance of the reverse projection check on simple toy examples. Second, the work [55] 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 have 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.

In terms of applications of such sampling techniques, members of the project-team have been working on two different subjects: random matrices models and adaptive techniques to compute large deviation rate functionals. The paper [16] was written by G. Ferré and D. Chafaï (Université Paris Dauphine, France), following the simple idea: the eigenvalues of random matrices are distributed according to Boltzmann–Gibbs measures, but researchers in this field do not use techniques from statistical physics for numerical investigations. The authors therefore used a Hamiltonian Monte Carlo algorithm to investigate numerically conjectures about random matrices and related Coulomb gases. The next step is to add constraints to these systems to understand better the behavior of random matrices with constraints and the large size limit of their spectra (the algorithm mentioned above to sample probability measures supported on submanifolds may be useful in this context). The work [19] focuses on computing free energies and entropy functions, as they arise in large deviations theory, through adaptive techniques. It is actually in the spirit of techniques used in mathematical finance, adapted to the statistical mechanics context, and enriched with new estimators based on variational representations of entropy functions. These tools have been pioneered by H. Touchette (Stellenbosch University, South Africa), with whom the paper was written by G. Ferré.

6.2.2. Sampling of the configuration space: numerical analysis

Concerning the numerical analysis of sampling techniques of probability measures on the configuration space, let us mention three works.

First, in [44], G. Ferré and G. Stoltz study the numerical errors that arise when a stochastic differential equation (SDE) is discretized in order to compute scaled cumulant functions (or free energy) and ergodic properties of Feynman–Kac semigroups. These quantities naturally arise in large deviations theory, for estimating probabilities of rare events. This analysis is made difficult by the nonlinear (mean field) feature of the dynamics at hand. The obtained estimates generalize previous results on the numerical analysis of ergodic properties of discretized SDEs. As a theoretical extension of the previous work, the purpose of the work [43] by G. Ferré and G. Stoltz, in collaboration with M. Rousset (Inria Rennes, France), is to provide further theoretical investigations on the long time behavior of Feynman–Kac semigroups. More precisely, it aims at giving practical criteria for these nonlinear semigroups to have a limit, and makes precise in which sense this limit is to be understood. This was an open problem so far for systems evolving in unbounded configuration spaces, which was addressed through Lyapunov function techniques. Although theoretical, these results are of practical importance since, if these dynamics do not have a well-defined long time behavior, it is hopeless to try to compute rare events.

Finally, together with C. Andrieu (Univ. Bristol, United-Kingdom), A. Durmus (ENS Saclay, France) and N. Nüsken (Univ. Potsdam, Germany), J. Roussel derived in [32] spectral gap estimates for several Piecewise Deterministic Markov Processes (PDMPs), namely the Randomized Hamiltonian Monte Carlo, the Zig-Zag process and the Bouncy Particle Sampler. The hypocoercivity technique provides estimates with explicit dependence on the parameters of the dynamics. Moreover the general framework considered allows to compare quantitatively the bounds found for the different methods. Such PDMDs are currently more and more used as efficient sampling tools, but their theoretical properties are still not yet well understood.

6.2.3. 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. Members of the project-team are following two numerical approaches to sample

metastable trajectories: the accelerated dynamics *à la* A.F. Voter and the adaptive multilevel splitting (AMS) technique to sample reactive paths between metastable states.

Concerning the mathematical analysis of the accelerated dynamics, in [50], T. Lelièvre reviews the recent mathematical approaches to justify these numerical methods, using the notion of quasi-stationary distribution. Moreover, in [49], T. Lelièvre together with D. Le Peutrec (Université de Paris Saclay, France) and G. Di Gesu and B. Nectoux (TU Wien, Austria) give an overview of the results obtained during the PhD of B. Nectoux. Using the quasi-stationary distribution approach and tools from semi-classical analysis, one can justify the use of kinetic Monte Carlo models parametrized by the Eyring-Kramers formulas to describe exit events from metastable states, for the overdamped Langevin dynamics. Concerning the implementation, in [22], F. Hédin and T. Lelièvre test the Generalized Parallel Replica algorithm to biological systems, and obtain strong linear scalability, providing up to 70% of the maximum possible speedup on several hundreds of CPUs. The "Parallel Replica" (ParRep) dynamics is known for allowing to simulate very long trajectories of metastable Langevin dynamics in the materials science community, but it relies on assumptions that can hardly be transposed to the world of biochemical simulations. The later developed "Generalized ParRep" variant solves those issues, and it had not been applied to significant systems of interest so far. Finally, let us mention the work [27] where T. Lelièvre together with J. Reygner (Ecole des Ponts, France) and L. Pillaud-Vivien (Inria Paris, France) analyze mathematically the Fleming-Viot particle process in the simple case of a finite state space. This Fleming-Viot particle process is a key ingredient of the Generalized ParRep algorithm mentioned above, in order to both approximate the convergence time to the quasi-stationary distribution, and to efficiently sample it.

Concerning the AMS technique, in [36], T. Lelièvre and C.-E. Bréhier (ENS Lyon, France) test new importance functions to compute rare events associated with the law of the solution to a stochastic differential equation at a given fixed time. This can be used for example to estimate the rate functional for large deviation principle applied to time averages.

6.2.4. Coarse-graining

In two related works, members of the project-team have studied the quality of the effective dynamics derived from a high dimension stochastic differential equation on a few degrees of freedom, using a projection approach *à la Mori-Zwanzig*. More precisely, in [48], F. Legoll, T. Lelièvre and U. Sharma obtain precise error bounds in the case of non reversible dynamics. This analysis also aims at discussing what is a good notion of mean force for non reversible systems. In [53], T. Lelièvre together with W. Zhang (ZIB, Germany) extend previous results on pathwise error estimates for such effective dynamics to the case of nonlinear vectorial reaction coordinates.

Once a good coarse-grained model has been obtained, one can try to use it in order to get a better integrator of the original dynamic in the spirit of a predictor-corrector method. In [52], T. Lelièvre together with G. Samaey and P. Zielinski (KU Leuven, Belgium) analyze such a micro-macro acceleration method for the Monte Carlo simulation of stochastic differential equations with time-scale separation between the (fast) evolution of individual trajectories and the (slow) evolution of the macroscopic function of interest.

6.3. Homogenization

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

6.3.1. Deterministic non-periodic systems

In homogenization theory, members of the project-team have pursued their ongoing systematic study of perturbations of periodic problems (by local and nonlocal defects). This has been done in two different directions.

For linear elliptic equations, C. Le Bris has written, in collaboration with X. Blanc (Paris Diderot, France) and P.-L. Lions (Collège de France, France), two manuscripts that present a more versatile proof of the existence of a corrector function for periodic problems with local defects, and also extend the results: the first manuscript [34] addresses the case of an equation (or a system) in divergence form, while the second manuscript [12] extends the analysis to advection-diffusion equations.

Second, they have also provided more details on the quality of approximation achieved by their theory. The fact that a corrector exists with suitable properties allows one to quantify the rate of convergence of the two-scale expansion using that corrector to the actual exact solution, as the small homogenization parameter ε vanishes. These works by C. Le Bris, in collaboration with X. Blanc and M. Josien (and in the context of the PhD thesis of the latter), will be presented in a series of manuscripts in preparation. The precise results have been announced in [11] and proven in [33]. A related study [47] has been performed by M. Josien and addresses issues regarding periodic Green functions.

Also in the context of homogenization theory, C. Le Bris and F. Legoll have initiated a collaboration with R. Cottereau (Ecole Centrale and now CNRS Marseille, France). The topic is in some sense a follow-up on both an earlier work of R. Cottereau and the series of works completed by C. Le Bris and F. Legoll in collaboration with K. Li and next S. Lemaire over the years. Schematically, the purpose of the work is to determine the homogenized coefficient for a medium without explicitly performing a homogenization approach nor using a MsFEM type approach. In earlier works, an approximation approach, somewhat engineering-style, was designed. The purpose now is to examine the performance of this approach in the context of the so-called Arlequin method, a very popular method in the mechanical engineering community. One couples a sub-region of the medium where a homogeneous model is employed, along with a complementary sub-region where the original multiscale model is solved explicitly. The coupling is performed using the Arlequin method. Then, one optimizes a suitable criterion so that optimization leads to an homogeneous sub-region indeed described by the homogenized coefficient seeked for. Some numerical analysis questions, together with practical perspectives for computational enhancements of the approach, are currently examined.

Finally, C. Le Bris has informally participated into the supervision of the master thesis of S. Wolf (Ecole Normale Supérieure, Paris, France), and in this context performed some works in interaction with the student and X. Blanc. The purpose is to investigate perturbations of periodic homogenization problems when the perturbation is geometric in nature. The test case considered is that of a domain perforated by holes the locations of which are not necessarily periodic, but only periodic up to a local perturbation. The results proven, on the prototypical Poisson equation, are natural extensions of the celebrated results by J.-L. Lions published in the late 1960s for the periodic case. This provides a proof of concept, showing that perturbations of a periodic geometry are also possible, a fact that will be more thoroughly investigated in the near future within the above mentioned collaboration.

6.3.2. Stochastic homogenization

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

Using standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the whole space $\mathbb{R}^d$. This equation is therefore delicate and expensive to solve. A standard approach consists in truncating the space $\mathbb{R}^d$ to some bounded domain, on which the corrector problem is numerically solved.

In collaboration with B. Stamm (Aachen University, Germany) and S. Xiang (now also at Aachen University, Germany), E. Cancès, V. Ehrlacher and F. Legoll have studied, both from a theoretical and a numerical standpoints, new alternatives for the approximation of the homogenized matrix. They all rely on the use of an embedded corrector problem, previously introduced by the authors, where a finite-size domain made of the highly oscillatory material is embedded in a homogeneous infinite medium whose diffusion coefficients have to be appropriately determined. In [40], they have shown that the different approximations introduced all converge to the homogenized matrix of the medium when the size of the embedded domain goes to infinity. In [41], they present an efficient algorithm for the resolution of such problems for particular heterogeneous materials, based on the reformulation of the embedded corrector problem as an integral equation, which is discretized using spherical harmonics and solved using the fast multipole method.

Besides the averaged behavior of the oscillatory solution u_ε on large space scales (which is given by its homogenized limit), a question of interest is to describe how u_ε fluctuates. This question is investigated in the PhD thesis of P.-L. Rothé, both from a theoretical and a numerical viewpoints. First, theoretical results

have been obtained for a weakly stochastic setting (where the coefficient is the sum of a periodic coefficient and a small random perturbation). It has been shown that, at the first order and when ε is small, the localized fluctuations (characterized by a test function g) of u_ε are Gaussian. The corresponding variance depends on the localization function g, on the right-hand side f of the problem satisfied by u_ε, and on a fourth order tensor Q which is defined in terms of the corrector. Since the corrector function is challenging to compute, so is Q. A numerical approach has hence been designed to approximate Q and its convergence has been proven. Second, numerical experiments in more general settings (i.e. full stochastic case) following the same approach have been performed. The results are promising, and consistent with the theoretical results obtained in the weakly stochastic setting. These results are collected in a manuscript in preparation.

In collaboration with T. Hudson (University of Warwick, United Kingdom), F. Legoll and T. Lelièvre have considered in [46] a scalar viscoelastic model in which the constitutive law is random and varies on a lengthscale which is small relative to the overall size of the solid. Using stochastic two-scale convergence, they have obtained the homogenized limit of the evolution, and have demonstrated that, under certain hypotheses, the homogenized model exhibits hysteretic behaviour which persists under asymptotically slow loading. This work is motivated by rate-independent stress-strain hysteresis observed in filled rubber.

6.3.3. Multiscale Finite Element approaches

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

During the year, several research tracks have been pursued in this general direction.

The final writing of the various works performed in the context of the PhD thesis of F. Madiot is still ongoing. The issues examined there are on the one hand the application (and adequate adjustment) of MsFEM approaches to the case of an advection-diffusion equation with a dominating convection term posed in a perforated domain, and on the other hand some more general study of a numerical approach based, again in the case of convection-dominated flows, on the introduction of the invariant measure associated to the problem. The final version of the two manuscripts describing the efforts in each of these directions should be completed in a near future.

The MsFEM approach uses a Galerkin approximation of the problem on a pre-computed basis, obtained by solving local problems mimicking the problem at hand at the scale of mesh elements, with carefully chosen right-hand sides and boundary conditions. The initially proposed version of MsFEM uses as basis functions the solutions to these local problems, posed on each mesh element, with null right-hand sides and with the coarse P1 elements as Dirichlet boundary conditions. Various improvements have next been proposed, such as the *oversampling* variant, which solves local problems on larger domains and restricts their solutions to the considered element. In collaboration with U. Hetmaniuk (University of Washington in Seattle, USA), C. Le Bris, F. Legoll and P.-L. Rothé have introduced and studied a MsFEM method improved differently. They have considered a variant of the classical MsFEM approach with enrichments based on Legendre polynomials, both in the bulk of the mesh elements and on their interfaces. A convergence analysis of this new variant has been performed. Promising numerical results have been obtained. These results are currently being collected in a manuscript in preparation.

One of the perspectives of the team, through the PhD thesis of A. Lesage, is the development of Multiscale Finite Element Methods for thin heterogeneous plates. The fact that one of the dimension of the domain of interest scales as the typical size of the heterogeneities within the material induces theoretical and practical difficulties that have to be carefully taken into account. The first steps of the work of V. Ehrlacher, F. Legoll and A. Lesage, in collaboration with A. Lebée (École des Ponts) have consisted in studying the homogenized limit (and the two-scale expansion) of problems posed on thin heterogeneous plates. The case of a diffusion equation has been first dealt with, while the more challenging case of elasticity is currently under study.

6.4. 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 real materials flows, multi-phase fluids such as suspensions of particles or stratified air-water flows in particular, and
- to propose efficient algorithms for the computation of flow solutions, mainly for the many applications in the hydraulic engineering context.

Concerning the first point, new results have been obtained in collaboration with A. Caboussat (HEG, Switzerland) and M. Picasso (EPFL, Switzerland), in the framework of the SEDIFLO project (funded by ANR) and of Arwa Mrad PhD thesis at EPFL. In [13], they have shown numerically inability of some classical incompressible density-dependent Navier-Stokes equations to take into account some multiphase concentration effects in a prototypical set-up of fluvial erosion (in comparison with physical experiments). Hence the need for *new* models, that better describe complex flows associated with heterogeneities in the fluid microstructure. Concerning the second point, new results have been obtained in collaboration with M. Grepl and K. Veroy (Aachen, Germany) regarding the numerical reduction of transport models for data assimilation [25], in the framework of M. Kaercher PhD thesis at Aachen.

MEMPHIS Project-Team

7. New Results

7.1. Hybrid FOM/ROM simulations for turbulent flows

We present below results concerning the application of the hybrid FOM/ROM method to a realistic problem in CFD. The purpose of the study is to investigate the behavior of the flow past a car for several front bumper configurations. We here resort to Free-Form Deformation (FFD) based on two parameters to determine a satisfactory parametrization of all possible configurations, and we consider a steady RANS solver at $\mathrm{Re} = 4.87 \cdot 10^6$ with Spalart-Allmaras turbulence model to simulate the flow. Simulations are performed in collaboration with OPTIMAD (http://www.optimad.it/) exploiting the methodology proposed in [15].

Figure 6 (left) shows the domain decomposition; in the blue region we solve the Full-Order model, while in the outer region we rely on a POD-Galerkin Reduced Order model. The partitioning is obtained adaptively using the algorithm described in [15]. Figure 6 (right) shows the flow prediction error relative to dynamic pressure for the worst-case parameter: the proposed method leads to 2% accurate results with a speed-up compared to the full-order model of 8.

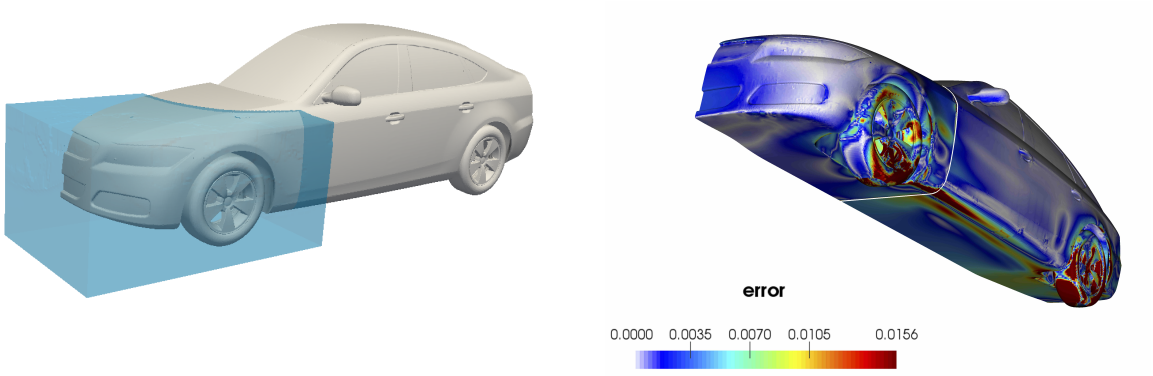


Figure 6. hybrid FOM/ROM approach; application to RANS modelling of the flow around a car.

7.2. All-speed multi-material schemes

We are interested in the development of numerical models for phenomena involving fluid flows and elastic material deformations. We pursue a monolithic approach, which describes the behavior of each material (gas, liquid or solid) through a system of conservation laws and appropriate constitutive relationships. Our method is designed to handle both high-Mach and low-Mach regimes.

It is well-known that Godunov-type schemes are inadequate for low-Mach problems: first, they introduce an eccessive amount of numerical artificial viscosity; second, they require the enforcement of a CFL stability condition which leads to unpractical time steps. For this reason, we resort to the relaxation method proposed in [36], to derive a novel discretization scheme which can be applied to problems characterized by a broad range of Mach numbers. As opposed to [36], we propose in [1] to treat the advective term implicitly.

Figure 7 shows results for a quasi 1D de Laval nozzle problem in water: the flow is low-Mach and almost incompressible. In the present simulation, we impose at the inlet the total pressure $P_{\rm tot} = 10{\rm Pa}$ and the absolute temperature $T = 280K$ and at the outlet the pressure $p_{\rm out} = 1{\rm Pa}$. Figure 7 (center) shows results for the explicit scheme proposed in [36], while Figure 7 (right) shows results of our implicit scheme; for the explicit schemes, we impose the acoustic CFL $\nu_{\rm ac} = 0.4$, while for the implicit scheme, we consider $\nu_{\rm ac} = 100$. We observe that our method outperforms the method in [36].

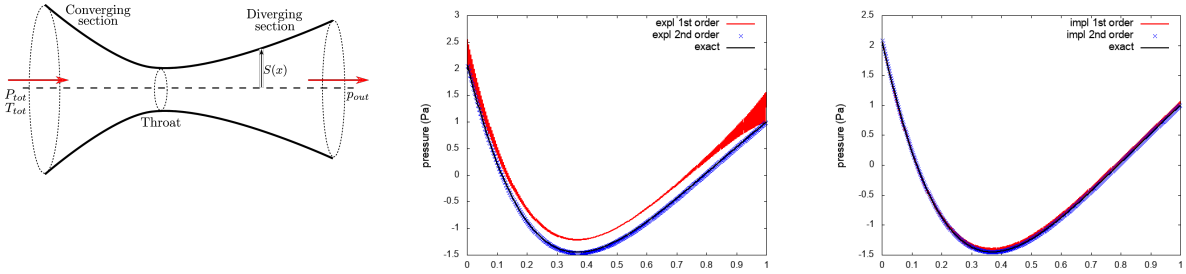


Figure 7. all-speed relaxation scheme. Left: de Laval nozzle. Center: pressure distribution predicted by the explicit method in [36] ($\nu_{\rm ac} = 0.4$). Right: pressure distribution predicted by the implicit method proposed in [1] ($\nu_{\rm ac} = 100$).

7.3. Thermal convection on a hemisphere

Hamid Kellay (LOMA) performs a physical experiment using a half soap bubble heated at the equator. This device allows to study thermal convection and the movement of large scale structures on the surface of the bubble. The results show strong similarities with atmospheric flows on the earth. In particular large vortical structures on the half bubble and tropical cyclones in the atmosphere have the same dynamics.

Using a stereographic transform we solve Navier-Stokes equations on the half bubble and get very good agreement with the experiment. In addition we find that the Nusselt and Reynolds numbers varify scaling laws quite close to the scaling law given in the literature for Rayleigh-Bénard convection: ${\rm Nu} \propto {\rm Ra}^{0.31}$ and ${\rm Re} \propto {\rm Ra}^{1/2}$. Finally a Bolgieno regime is found with scaling as $Ra^{-1/4}$.

Adding the rotation like on the earth we show that the rotation changes the nature of turbulent fluctuations and a new scaling regime is obtained for the temperature field.

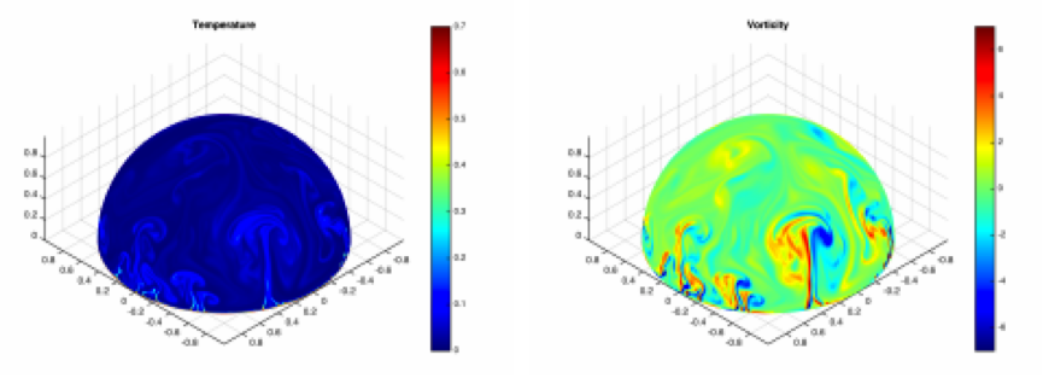


Figure 8. Temperature (left) and vorticity (right) fields at the stationary state for $Ra = 3.10^8$ and $Pr = 7$. Plumes move upward and interact with each other.

MEPHYSTO-POST Team

4. New Results

4.1. Exponential time-decay for discrete Fokker–Planck equations

G. Dujardin and his coauthors proposed and studied in [22] several discrete versions of homogeneous and inhomogeneous one-dimensional Fokker-Planck equations. They proved in particular, for these discretizations of velocity and space, the exponential convergence to the equilibrium of the solutions, for time-continuous equations as well as for time-discrete equations. Their method uses new types of discrete Poincaré inequalities for a "two-direction" discretization of the derivative in velocity. For the inhomogeneous problem, they adapted hypocoercive methods to the discrete level.

4.2. Energy preserving methods for nonlinear Schrödinger equations

G. Dujardin and his coauthors have revisited and extended relaxation methods for nonlinear Schrödinger equations (NLS). The classical relaxation method for NLS is an energy preserving method and a mass preserving method. Moreover, it is only linearly implicit. A first proof of the second order accuracy was achieved in [14]. Moreover, the method was extended to enable to treat noncubic nonlinearities, nonlocal nonlinearities, as well as rotation terms. The resulting methods are still energy preserving and mass preserving. Moreover, they are shown to have second order accuracy numerically. These new methods are compared with fully implicit, mass and energy preserving methods of Crank and Nicolson.

4.3. Diffusive and superdiffusive behavior in one-dimensional chains of oscillators

In order to understand abnormally diffusive phenomena which are physically observed in nanotube technologies, one mathematical approach consists in starting from deterministic system of Newtonian particles, and then perturb this system with a stochastic component which provides enough ergodicity to the dynamics. It is already well known that these stochastic chains model correctly the behavior of the conductivity [24]. In [1], [2] (published in Communications in Mathematical Physics) 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 [31], [32]. Moreover, in [2], the authors manage to treat rigorously, for the first time, the case of an anharmonic potential: more precisely, they consider a small quartic anharmonicity and show that the result obtained in the harmonic (linear) case persists up to some small critical value of the nonlinear perturbation.

4.4. Microscopic description of moving interfaces

A large variety of models has been introduced to describe the evolution of a multiphase medium, *e.g.* the joint evolution of liquid and solid phases. These complex physical phenomena often feature absorbing phase transitions. For instance, the porous medium equation (PME)

$$\partial_t \rho = \mathrm{div}(\rho^{m-1}\, \nabla \rho), \tag{1}$$

where $m > 1$ is a constant and div and ∇ are the divergence and gradient operators in $\mathbb{R}^d$, describes the evolution of the density $\rho : \mathbb{R}^d \times \mathbb{R}_+ \to [0, 1]$ of an ideal gas flowing in a homogeneous medium. It is known that, starting from an initial density ρ_0 with compact support, the solution $\rho(x, t)$ is nonnegative and has compact support in the space variable for each positive t. Thus there are interfaces separating the regions where ρ is positive from those where it is zero.

In one submitted paper in collaboration with O. Blondel, C. Cancès, and M. Sasada, we have derived the PME (1) from a degenerate and conservative dynamics in [15], for any integer $m > 1$. More precisely we improved the results previously obtained in [26], since we allow the solutions to feature moving interfaces, namely the initial condition may vanish. This moving boundary was not well apprehended at the microscopic level. Its rigorous definition is indeed very delicate, and its behavior (such that its speed, or fluctuation), as well as the relationship between the microscopic and macroscopic boundaries, are challenging questions that we aim to tackle in a near future.

When $m < 1$, equation (1) is called fast diffusion equation. In a recent collaborative work (submitted) with O. Blondel, C. Erignoux and M. Sasada [16], we derive such a fast diffusion equation in dimension one from an interacting particle system belonging to the class of conserved lattice gases with active-absorbing phase transition [30]. The microscopic dynamics is very constrained: in a few words, a particle can jump to the right (resp. left) empty neighboring site if and only if it has a particle to its left (resp. right) neighboring site. This model is really complex: the state space is divided into transient states, absorbing states and ergodic states. Depending on the initial number of particles, the transient good configurations will lead to the ergodic component and the transient bad configurations will be absorbed to an inactive state. Because of the jump constraint, there are two distinct regimes for the macroscopic behavior. Either the macroscopic density is larger than $\frac{1}{2}$, in which case the system behaves diffusively, or the density is lower than $\frac{1}{2}$, in which case the system freezes rapidly.

The interfaces between these two phases propagate as particles from the supercritical phase ($\rho > \frac{1}{2}$) diffuse towards the subcritical phase ($\rho < \frac{1}{2}$). We expect that the macroscopic density profile evolves under the diffusive scaling according to the Stefan problem

$$\partial_t \rho = \Delta\left(G(\rho)\right) \qquad \text{where } G(\rho) = \tfrac{2\rho-1}{\rho}\, \mathbf{1}_{\rho>\frac{1}{2}}. \tag{2}$$

The microscopic derivation of such Stefan problems is a well known difficult problem, only partially solved [27], [29]. In [16] we treat the liquid part of the problem (*i.e.* when the initial profiles ρ_0 are uniformly larger than the critical density $\frac{1}{2}$) and we provide a refined estimation of the time needed by the system to enter into the ergodic state. Then, we show that the macroscopic density profile evolves under the diffusive time scaling according to (1) with $m = -1$. The extension to more general initial profiles is our next goal.

4.5. Stability analysis of a Vlasov-Wave system

S. De Bièvre and his co-authors introduced and studied a kinetic equation of the Vlasov-Wave type, which arises in the description of the behavior of a large number of particles interacting weakly with an environment, composed of an infinite collection of local vibrational degrees of freedom, modeled by wave equations. They use variational techniques to establish the existence of large families of stationary states for this system, and analyze their stability [8].

4.6. Orbital stability in the presence of symmetries

With S. Rota Nodari, S. De Bièvre considered the orbital stability of relative equilibria of Hamiltonian dynamical systems on Banach spaces, in the presence of a multi-dimensional invariance group for the dynamics [9]. They proved a persistence result for such relative equilibria, presented a generalization of the Vakhitov-Kolokolov slope condition to this higher dimensional setting, and showed how it allows to prove the local coercivity of the Lyapunov function, which in turn implies orbital stability. The method was applied to study the orbital stability of relative equilibria of nonlinear Schrödinger and Manakov equations. It extends and clarifies the approach of Grillakis-Shatah-Strauss.

4.7. Measuring nonclassicality of bosonic field quantum state

S. De Bièvre and his collaborators introduced a new distance-based measure for the nonclassicality of the states of a bosonic field, which outperforms the existing such measures in several ways [17]. They defined for that purpose the operator ordering sensitivity of the state which evaluates the sensitivity to operator ordering of the Renyi entropy of its quasi-probabilities and which measures the oscillations in its Wigner function. Through a sharp control on the operator ordering sensitivity of classical states they obtained a precise geometric image of their location in the density matrix space allowing them to introduce a distance-based measure of nonclassicality. They analyze the link between this nonclassicality measure and a recently introduced quantum macroscopicity measure, showing how the two notions are distinct.

4.8. The Cauchy problem for the Landau–Lifshitz–Gilbert equation in BMO and self-similar solutions

A. de Laire and S. Gutierrez established in [19] a global well-posedness result for the Landau–Lifshitz equation with Gilbert damping, provided that the BMO semi-norm of the initial data is small. As a consequence, they deduced the existence of self-similar solutions in any dimension. Moreover, in the one-dimensional case, they characterized the self-similar solutions when the initial data is given by some ($\S^2$-valued) step function and established their stability. They also showed the existence of multiple solutions if the damping is strong enough.

4.9. The Sine–Gordon regime of the Landau–Lifshitz equation with a strong easy-plane anisotropy

It is well-known that the dynamics of biaxial ferromagnets with a strong easy-plane anisotropy is essentially governed by the Sine-Gordon equation. A. de Laire and P. Gravejat provided in [10] a rigorous justification to this observation. More precisely, they showed the convergence of the solutions to the Landau-Lifshitz equation for biaxial ferromagnets towards the solutions to the Sine-Gordon equation in the regime of a strong easy-plane anisotropy. This result holds for solutions to the Landau–Lifshitz equation in high order Sobolev spaces. They also provided an alternative proof for local well-posedness in this setting by introducing high order energy quantities with better symmetrization properties. Then they derived the convergence from the consistency of the Landau–Lifshitz equation with the Sine-Gordon equation by using well-tailored energy estimates. As a by-product, they also obtained a further derivation of the free wave regime of the Landau–Lifshitz equation.

4.10. Mutual information of wireless channels and block-Jacobi ergodic operators

In telecommunication models the quality of the transferred data is assessed through the entropy of the channel, a theoretical quantity that is usually not computable in practice. W. Hachem, A. Hardy and S. Shamai prove in [23] that one can relate this quantity for a large class of models involving several antennas (MIMO) to the equilibrium measure of a matrix valued Markov chain associated with the model, and so does its asymptotic behavior when the signal-noise-ratio parameter becomes large. By means of ergodicity results, this yields estimates for these quantities that are implementable faster than the naive estimators.

4.11. DLR equations and rigidity for the Sine-beta process

The Sine-beta process is a universal object appearing in the study of large Hermitian random matrices and statistical systems in a logarithmic interaction, such as low dimensional Coulomb gases. However, the only description available yet relied on a rather complicated and non-physical system of coupled stochastic differential equations. In [21], D. Dereudre, A. Hardy, T. Leblé and M. Maïda obtain a statistical physic interpretation of the Sine-beta process as probability measure on infinite configurations of points described by means of the DLR formalism. This allows to obtain more information on the Sine-beta process: for instance, it is rigid, it is tolerant, and the number of particles in a compact box has gaussian fluctuations as the box becomes large.

4.12. Time-frequency transforms of white noises and Gaussian analytic functions

In signal processing, an important challenge is to be able to separate signals from ambient noises. In time-frequency analysis, this problem reduces to identify what is the spectrogram of a white noise to derive statistical tests in order to decide if some partial signal is noise or not. P. Fandrin recently put forward that the understanding of the zeros of the spectrograms would be already an important step by analyticity of the spectrograms. R. Bardenet and A. Hardy observed in [13] that there is a canonical way to identify the zeros of the usual white noise transforms associated to classical spectrograms and zeroes of Gaussian analytic functions associated with classical orthogonal polynomials in the background. In particular the zeros satisfy some invariance properties leading to computable correlation functions. In specific cases, one can identify some transforms whose zeros form a determinantal point process, in which case all the statistics of interests can be computed explicitly and this allows an exact numerical treatment.

4.13. Energy of the Coulomb gas on the sphere at low temperature

In relation to the 7th Smale problem, which is about finding polynomial time algorithm to produce well spread configuration of points on the sphere in a quantified manner, C. Beltran and A. Hardy proved in [4] that the Coulomb gas on the sphere at a temperature proportional to the inverse number of points in a configuration reaches the numerical precision required by this problem. We however did not discuss yet the algorithmic procedure, which is currently in investigation by A. Hardy and M. Simon.

4.14. Polynomial ensembles and recurrence coefficients

Determinantal point processes can be of important use in applications as soon as one is interested in producing configurations of well spread points on an arbitrary space. A class of determinantal point processes on the real line that has been extensively studied recently are the so-called polynomial ensembles. A. Hardy gathered in [11] several results concerning these models in relation to the recurrent coefficients associated with the orthogonal polynomials hidden in the background.

4.15. Concentration for Coulomb gases and Coulomb transport inequalities

The convergence of the Coulomb gas, which is a statistical gas of charged particles in an electrostatic interaction, towards its limiting distribution as the number of particles goes to infinity is a result which is part of the folklore of potential theory. The speed at which this convergence arise, which can be assessed through concentration of measure estimates in, say, the Wasserstein-Kantorovich metric, are however new results obtained by D. Chafaï, A. Hardy and M. Maïda in [7]. One of the main ingredient was to develop transport inequalities associated with the Coulomb interaction.

MINGUS Project-Team

7. New Results

7.1. Highly-oscillatory problems

7.1.1. Highly-oscillatory problems with time-dependent vanishing frequency

In the analysis of highly-oscillatory evolution problems, it is commonly assumed that a single frequency is present and that it is either constant or, at least, bounded from below by a strictly positive constant uniformly in time. Allowing for the possibility that the frequency actually depends on time and vanishes at some instants introduces additional difficulties from both the asymptotic analysis and numerical simulation points of view. This work [27] is a first step towards the resolution of these difficulties. In particular, P. Chartier, M. Lemou, F. Méhats and G. Vilmart show that it is still possible in this situation to infer the asymptotic behaviour of the solution at the price of more intricate computations and we derive a second order uniformly accurate numerical method.

7.1.2. Uniformly accurate methods for Vlasov equations with non-homogeneous strong magnetic field

In this paper [26], the authors P. Chartier, N. Crouseilles, M. Lemou, F. Méhats and X. Zhao consider the numerical solution of highly-oscillatory Vlasov and Vlasov-Poisson equations with non-homogeneous magnetic field. Designed in the spirit of recent uniformly accurate methods, our schemes remain insensitive to the stiffness of the problem, in terms of both accuracy and computational cost. The specific difficulty (and the resulting novelty of our approach) stems from the presence of a non-periodic oscillation, which necessitates a careful ad-hoc reformulation of the equations. Our results are illustrated numerically on several examples.

7.1.3. Uniformly accurate time-splitting methods for the semiclassical linear Schrödinger equation

The paper [8] is devoted to the construction of numerical methods which remain insensitive to the smallness of the semiclassical parameter for the linear Schrödinger equation in the semiclassical limit. We specifically analyse the convergence behavior of the first-order splitting. Our main result is a proof of uniform accuracy. The authors illustrate the properties of our methods with simulations. Philippe Chartier, Loïc Le Treust, Florian Méhats then illustrate the properties of the methods with simulations.

7.1.4. Numerical methods for the two-dimensional Vlasov-Poisson equation in the finite Larmor radius approximation regime

In this paper [7], the authors P. Chartier, N. Crouseilles and X. Zhao consider the numerical methods for solving the two-dimensional Vlasov-Poisson equation in the finite Larmor radius approximation regime. The model describes the behaviour of charged particles under a strong external magnetic field and the finite Larmor radius approximation. We discretise the equation under Particle-in-Cell method, where the characteristics equations are highly oscillatory system in the limit regime. We apply popular numerical integrators including splitting methods, multi-revolution composition methods, two-scale formulation method and limit solver to integrate the characteristics. Dissuasions are made to highlight the strength and drawback of each method. Numerical experiments are done, and comparisons on the accuracy, efficiency and long-time behaviour of the methods are made, aiming to suggest the method with the best performance for the problem.

7.1.5. A new class of uniformly accurate numerical schemes for highly oscillatory evolution equations

In [9], we introduce a new methodology to design uniformly accurate methods for oscillatory evolution equations. The targeted models are envisaged in a wide spectrum of regimes, from non stiff to highly oscillatory. Thanks to an averaging transformation, the stiffness of the problem is softened, allowing for standard schemes to retain their usual orders of convergence. Overall, high order numerical approximations are obtained with errors and at a cost independent of the regime.

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

In [2], we introduce efficient and robust exponential-type integrators for Klein-Gordon equations which resolve the solution in the relativistic regime as well as in the highly-oscillatory non-relativistic regime without any step-size restriction, and under the same regularity assumptions on the initial data required for the integration of the corresponding limit system. In contrast to previous works we do not employ any asymptotic/multiscale expansion of the solution. This allows us derive uniform convergent schemes under far weaker regularity assumptions on the exact solution. In particular, the newly derived exponential-type integrators of first-, respectively, second-order converge in the non-relativistic limit to the classical Lie, respectively, Strang splitting in the nonlinear Schrödinger limit.

7.1.7. A micro-macro method for a kinetic graphene model in one-space dimension

In [29], for the one space dimensional semiclassical kinetic graphene model recently introduced in the literature, we propose a micro-macro decomposition based numerical approach, which reduces the computational dimension of the nonlinear geometric optics method based numerical method for highly oscillatory transport equation developed in a previous work. The method solves the highly oscillatory model in the original coordinate, yet can capture numerically the oscillatory space-time quantum solution pointwisely even without numerically resolving the frequency. We prove that the underlying micro-macro equations have smooth (up to certain order of derivatives) solutions with respect to the frequency, and then prove the uniform accuracy of the numerical discretization for a scalar model equation exhibiting the same oscillatory behavior. Numerical experiments verify the theory.

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

In [12], 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.

7.1.9. Symmetric high order Gautschi-type exponential wave integrators pseudospectral method for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime

In [19], a group of high order Gautschi-type exponential wave integrators (EWIs) Fourier pseudospectral method are proposed and analyzed for solving the nonlinear Klein-Gordon equation (KGE) in the nonrelativistic limit regime, where a parameter which is inversely proportional to the speed of light, makes the solution propagate waves with wavelength in time and in space. With the Fourier pseudospectral method to discretize the KGE in space, we propose a group of EWIs with designed Gautschi's type quadratures for the temporal integrations, which can offer any intended even order of accuracy provided that the solution is smooth enough, while all the current existing EWIs offer at most second order accuracy. The scheme is explicit, time symmetric and rigorous error estimates show the meshing strategy of the proposed method is time step and

mesh size as, which is optimal among all classical numerical methods towards solving the KGE directly in the limit regime, and which also distinguish our methods from other high order approaches such as Runge-Kutta methods which require . Numerical experiments with comparisons are done to confirm the error bound and show the superiority of the proposed methods over existing classical numerical methods.

7.1.10. On the rotating nonlinear Klein-Gordon equation: non-relativistic limit and numerical methods

In [32], we consider both numerics and asymptotics aspects for the rotating nonlinear Klein Gordon (RKG) equation, an important PDE in relativistic quantum physics that can model a rotating galaxy in Minkowski metric and serves also as a model e.g. for a "cosmic superfluid". Firstly, we formally show that in the non-relativistic limit RKG converges to coupled rotating nonlinear Schrödinger equations (RNLS), which is used to describe the particle-antiparticle pair dynamics. Investigations of the vortex state of RNLS are carried out. Secondly, we propose three different numerical methods to solve RKG from relativistic regimes to non-relativistic regimes in polar and Cartesian coordinates. In relativistic regimes, a semi-implicit finite difference Fourier spectral method is proposed in polar coordinates where both rotation terms are diagonalized simultaneously. While in non relativistic regimes, to overcome the fast temporal oscillations, we adopt the rotating Lagrangian coordinates and introduce two efficient multiscale methods with uniform accuracy, i.e., the multi revolution composition method and the exponential integrator. Various numerical results confirm (uniform) accuracy of our methods. Simulations of vortices dynamics are presented.

7.2. Numerical schemes for Hamiltonian PDEs

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

In [14], we consider time discretizations of the Vlasov-HMF (Hamiltonian Mean-Field) equation based on splitting methods between the linear and non-linear parts. We consider solutions starting in a small Sobolev neighborhood of a spatially homogeneous state satisfying a linearized stability criterion (Penrose criterion). We prove that the numerical solutions exhibit a scattering behavior to a modified state, which implies a nonlinear Landau damping effect with polynomial rate of damping. Moreover, we prove that the modified state is close to the continuous one and provide error estimates with respect to the time stepsize.

7.2.2. Unconditional and optimal H^2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrödinger equation in high dimensions

In [17], The focus of this paper is 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 be at $O(h^2 + \tau^2)$ with mesh-size h and time step τ 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.

7.2.3. Modulation equations approach for solving vortex and radiation in nonlinear Schrödinger equation

In [16], we apply the modulation theory to study the vortex and radiation solution in the 2D nonlinear Schrödinger equation. The full modulation equations which describe the dynamics of the vortex and radiation separately are derived. A general algorithm is proposed to efficiently and accurately find vortices with prescribed values of energy and spin index. The modulation equations are solved by accurate numerical method. Numerical tests and simulations of radiation are given.

7.2.4. Unconditional L^∞-convergence of two compact conservative finite difference schemes for the nonlinear Schrödinger equation in multi-dimensions

In [18], we are concerned with the unconditional and optimal L^∞-error estimates of two fourth-order (in space) compact conservative finite difference time domain schemes for solving the nonlinear Schrödinger equation in two or three space dimensions. The fact of high space dimension and the approximation via compact finite difference discretization bring difficulties in the convergence analysis. The two proposed schemes preserve the total mass and energy in the discrete sense. To establish the optimal convergence results without any constraint on the time step, besides the standard energy method, the cut-off function technique as well as a lifting technique are introduced. On the contrast, previous works in the literature often require certain restriction on the time step. The convergence rate of the proposed schemes are proved to be of $O(h^4 + \tau^2)$ with time step τ and mesh size h in the discrete L^∞-norm. The analysis method can be directly extended to other finite difference schemes for solving the nonlinear Schrödinger-type equations. Numerical results are reported to support our theoretical analysis, and investigate the effect of the nonlinear term and initial data on the blow-up solution.

7.2.5. Verification of $2D$x$2D$ and two-species Vlasov-Poisson solvers

Recently $1D$x$1D$ two-species Vlasov-Poisson simulations have been performed by the semi-Lagrangian method. Thanks to a classical first order dispersion analysis, we are able to check in [1] the validity of their simulations; the extension to second order is performed and shown to be relevant for explaining further details. In order to validate multi-dimensional effects, we propose a $2D$x$2D$ single species test problem that has true $2D$ effects coming from the sole second order dispersion analysis. Finally, we perform, in the same code, full $2D$x$2D$ non linear two-species simulations with mass ratio $\sqrt{0.01}$, and consider the mixing of semi-Lagrangian and Particle-in-Cell methods.

7.2.6. An exponential integrator for the drift-kinetic model

In [11], 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.

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

In [15], we consider the approximation of the ground state of the one-dimensional cubic nonlinear Schrödinger equation by a normalized gradient algorithm combined with linearly implicit time integrator, and finite difference space approximation. We show that this method, also called imaginary time evolution method in the physics literature, is con-vergent, and we provide error estimates: the algorithm converges exponentially towards a modified solitons that is a space discretization of the exact soliton, with error estimates depending on the discretization parameters.

7.3. Analysis of PDE

7.3.1. Bounds on the growth of high discrete Sobolev norms for the cubic discrete nonlinear Schrödinger equations on $h\mathbb{Z}$

In [22], we consider the discrete nonlinear Schrödinger equations on a one dimensional lattice of mesh h, with a cubic focusing or defocusing nonlinearity. We prove a polynomial bound on the growth of the discrete Sobolev norms, uniformly with respect to the stepsize of the grid. This bound is based on a construction of higher modified energies.

7.3.2. Existence and stability of traveling waves for discrete nonlinear Schrödinger equations over long times

In [23], we consider the problem of existence and stability of solitary traveling waves for the one dimensional discrete non linear Schrödinger equation (DNLS) with cubic nonlinearity, near the continuous limit. We construct a family of solutions close to the continuous traveling waves and prove their stability over long times. Applying a modulation method, we also show that we can describe the dynamics near these discrete traveling waves over long times.

7.3.3. Smoothing properties of fractional Ornstein-Uhlenbeck semigroups and null-controllability

In [20], we study fractional hypoelliptic Ornstein-Uhlenbeck operators acting on $L^2(\mathbb{R}^n)$ satisfying the Kalman rank condition. We prove that the semigroups generated by these operators enjoy Gevrey regularizing effects. Two byproducts are derived from this smoothing property. On the one hand, we prove the null-controllability in any positive time from thick control subsets of the associated parabolic equations posed on the whole space. On the other hand, by using the interpolation theory, we get global L^2 subelliptic estimates for the these operators.

7.3.4. Stable ground states for the HMF Poisson model

In [31], 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.

7.4. Dissipative problems

7.4.1. A formal series approach to the center manifold theorem

In [4], the author considers 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.

7.4.2. Analysis of an asymptotic preserving scheme for stochastic linear kinetic equations in the diffusion limit

In [21], we present an asymptotic preserving scheme based on a micro-macro decomposition for stochastic linear transport equations in kinetic and diffusive regimes. We perform a mathematical analysis and prove that the scheme is uniformly stable with respect to the mean free path of the particles in the simple telegraph model and in the general case. We present several numerical tests which validate our scheme.

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

In [28], 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 Δt 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 of the authors 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.

7.4.4. Time diminishing schemes (TDS) for kinetic equations in the diffusive scaling

In [28], we develop a new class of numerical schemes for collisional kinetic equations in the diffusive regime. The first step consists in reformulating the problem by decomposing the solution in the time evolution of an equilibrium state plus a perturbation. Then, the scheme combines a Monte Carlo solver for the perturbation with a Eulerian method for the equilibrium part, and is designed in such a way to be uniformly stable with respect to the diffusive scaling and to be consistent with the asymptotic diffusion equation. Moreover, since particles are only used to describe the perturbation part of the solution, the scheme becomes computationally less expensive - and is thus time diminishing (TDS) - as the solution approaches the equilibrium state due to the fact that the number of particles diminishes accordingly. This contrasts with standard methods for kinetic equations where the computational cost increases (or at least does not decrease) with the number of interactions. At the same time, the statistical error due to the Monte Carlo part of the solution decreases as the system approaches the equilibrium state: the method automatically degenerates to a solution of the macroscopic diffusion equation in the limit of infinite number of interactions. After a detailed description of the method, we perform several numerical tests and compare this new approach with classical numerical methods on various problems up to the full three dimensional case.

7.5. Stochastic PDE

7.5.1. Linearized wave turbulence convergence results for three-wave systems

In [30], E. Faou considers stochastic and deterministic three-wave semi-linear systems with bounded and almost continuous set of frequencies. Such systems can be obtained by considering nonlinear lattice dynamics or truncated partial differential equations on large periodic domains. We assume that the nonlinearity is small and that the noise is small or void and acting only in the angles of the Fourier modes (random phase forcing). We consider random initial data and assume that these systems possess natural invariant distributions corresponding to some Rayleigh-Jeans stationary solutions of the wave kinetic equation appearing in wave turbulence theory. We consider random initial modes drawn with probability laws that are perturbations of theses invariant distributions. In the stochastic case, we prove that in the asymptotic limit (small nonlinearity, continuous set of frequency and small noise), the renormalized fluctuations of the amplitudes of the Fourier modes converge in a weak sense towards the solution of the linearized wave kinetic equation around these Rayleigh-Jeans spectra. Moreover, we show that in absence of noise, the deterministic equation with the same random initial condition satisfies a generic Birkhoff reduction in a probabilistic sense, without kinetic description at least in some regime of parameters.

7.5.2. Large deviations for the dynamic Φ_d^{2n} model

In [5], 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 ρ and $\delta(\rho)$, respectively, with $0 < \rho, \delta(\rho) \ll 1$. We prove that, under the assumption that ρ 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 square-integrable 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.

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

In [3], 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 previously. The tools we develop are very general and can be used to study many other examples of applications.

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

In [6], we are dealing with the validity of a large deviation principle for the two-dimensional Navier-Stokes equation, with periodic boundary conditions, perturbed by a Gaussian random forcing. We are here interested in the regime where both the strength of the noise and its correlation are vanishing, on a length scale ε and $\delta(\varepsilon)$, respectively, with $0 < \varepsilon, \delta(\varepsilon) \ll 1$. Depending on the relationship between ε and $\delta(\varepsilon)$ we will prove the validity of the large deviation principle in different functional spaces.

7.5.5. The Schrödinger equation with spatial white noise potential

In [13], we consider the linear and nonlinear Schrödinger equation with a spatial white noise as a potential in dimension 2. We prove existence and uniqueness of solutions thanks to a change of unknown originally used in a paper by Hairer and Labbé (2015) and conserved quantities.

MOKAPLAN Project-Team

6. New Results

6.1. Rank optimality for the Burer-Monteiro factorization

I. Waldspurger, A. Watersw

In [39], Numerically solving a large scale semidefinite program, in full generality, is a challenge: The complexity of generic algorithms blows up quickly with the size of the unknown matrix. Fortunately, in many situations, the solution of the program has low rank, and this can be exploited to achieve algorithmic speedups. The most classical way to do this is the Burer-Monteiro factorization, introduced in [77]. It consists in writing the unknown matrix as the product of low-rank factors, and optimizing the factors instead of the matrix itself. The first theoretical guarantees for this method appeared in [69], where it was shown that this strategy almost always succeeds when the size of the factors is of the order of the square root of the full matrix. In our article, we show that, up to a marginal improvement, this result is optimal: Contrarily to what numerical experiments might suggest, there exist situations where the method fails if the size of the factors is chosen smaller.

6.2. Representer theorems in variational problems

C. Boyer, A. Chambolle, Y. De Castro, V. Duval, F. De Gournay, P. Weiss

In [29], we have established a general principle which states that regularizing an inverse problem with a convex function yields solutions which are convex combinations of a small number of *atoms*. These atoms are identified with the extreme points and elements of the extreme rays of the regularizer level sets. An extension to a broader class of quasi-convex regularizers is also discussed. As a side result, we characterize the minimizers of the total gradient variation, describing the solutions of total variation problem as a superposition of indicator functions of simply connected sets. That result provides an explanation of the so-called *staircasing* phenomenon.

6.3. The Sliding Frank-Wolfe algorithm for Super-resolution Microscopy Imaging

Q. Denoyelle, V. Duval, G. Peyré, E. Soubies

In [32], we have studied the theoretical and numerical performance of the Sliding Frank-Wolfe, a novel optimization algorithm to solve the BLASSO sparse spikes super-resolution problem. The BLASSO is a continuous (*i.e.* off-the-grid or grid-less) counterpart to the well-known ℓ^1 sparse regularisation method (also known as LASSO or Basis Pursuit). Our algorithm is a variation on the classical Frank-Wolfe (also known as conditional gradient) which follows a recent trend of interleaving convex optimization updates (corresponding to adding new spikes) with non-convex optimization steps (corresponding to moving the spikes). Our main theoretical result is that this algorithm terminates in a finite number of steps under a mild non-degeneracy hypothesis. We then target applications of this method to several instances of single molecule fluorescence imaging modalities, among which certain approaches rely heavily on the inversion of a Laplace transform. Our second theoretical contribution is the proof of the exact support recovery property of the BLASSO to invert the 1-D Laplace transform in the case of positive spikes. On the numerical side, we conclude this paper with an extensive study of the practical performance of the Sliding Frank-Wolfe on different instantiations of single molecule fluorescence imaging, including convolutive and non-convolutive (Laplace-like) operators. This shows the versatility and superiority of this method with respect to alternative sparse recovery techniques.

6.4. Approximation of variational problems with a convexity constraint by PDEs of Abreu type

G. Carlier, T. Radice

In [31], motivated by some variational problems subject to a convexity constraint, we consider an approximation using the logarithm of the Hessian determinant as a barrier for the constraint. We show that the minimizer of this penalization can be approached by solving a second boundary value problem for Abreu's equation which is a well-posed nonlinear fourth-order elliptic problem. More interestingly, a similar approximation result holds for the initial constrained variational problem.

6.5. Variational methods for tomographic reconstruction with few views

M. Bergounioux, I. Abraham, R. Abraham, G. Carlier, E. Le Pennec, E. Trélat

In [16], we deal with a severe ill posed problem, namely the reconstruction process of an image during tomography acquisition with (very) few views. We present different methods that we investigated during the past decade. They are based on variational analysis. This is a survey paper and we refer to the quoted papers for more details.

6.6. A differential approach to the multi-marginal Schrödinger system

G. Carlier, M. Laborde

In [30], we develop an elementary and self-contained differential approach, in an L^∞ setting, for well-posedness (existence, uniqueness and smooth dependence with respect to the data) for the multi-marginal Schrödinger system which arises in the entropic regularization of optimal transport problems.

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

J-D. Benamou, V. Duval

In [15] we present an adaptation of the MA-LBR scheme to the Monge-Ampr`e 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.

6.8. Second order models for optimal transport and cubic splines on the Wasserstein space

J-D. Benamou, T. O. Gallouët, F-X. Vialard

On the space of probability densities, we extend in [28] the Wasserstein geodesics to the case of higher-order interpolation such as cubic spline interpolation. After presenting the natural extension of cubic splines to the Wasserstein space, we propose a simpler approach based on the relaxation of the variational problem on the path space. We explore two different numerical approaches, one based on multi-marginal optimal transport and entropic regularization and the other based on semi-discrete optimal transport.

6.9. An entropy minimization approach to second-order variational mean-field games

J-D. Benamou, G. Carlier, S. Di Marino, L. Nenna

In [26] we propose a new viewpoint on variational mean-field games with diffusion and quadratic Hamiltonian. We show the equivalence of such mean-field games with a relative entropy minimization at the level of probabilities on curves. We also address the time-discretization of such problems, establish Gamma-Convergence results as the time step vanishes and propose an efficient algorithm relying on this entropic interpretation as well as on the Sinkhorn scaling algorithm.

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

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

Starting from Brenier's relaxed formulation of the incompress-ible Euler equation in terms of geodesics in the group of measure-preserving diffeomorphisms, we propose in [27] a numerical method based on Sinkhorn's algorithm for the entropic regularization of optimal transport. We also make a detailed comparison of this entropic regular-ization with the so-called Bredinger entropic interpolation problem (see [1]). Numerical results in dimension one and two illustrate the feasibility of the method.

6.11. Testing Gaussian Process with Applications to Super-Resolution

J.-M. Azaïs, Y. De Castro, S. Mourareau

In [13], we introduce exact testing procedures on the mean of a Gaussian process X derived from the outcomes of ℓ_1-minimization over the space of complex valued measures. The process X can be thought as the sum of two terms: first, the convolution between some kernel and a target atomic measure (mean of the process); second, a random perturbation by an additive centered Gaussian process. The first testing procedure considered is based on a dense sequence of grids on the index set of X and we establish that it converges (as the grid step tends to zero) to a randomized testing procedure: the decision of the test depends on the observation X and also on an independent random variable. The second testing procedure is based on the maxima and the Hessian of X in a grid-less manner. We show that both testing procedures can be performed when the variance is unknown (and the correlation function of X is known). These testing procedures can be used for the problem of deconvolution over the space of complex valued measures, and applications in frame of the Super-Resolution theory are presented. As a byproduct, numerical investigations may demonstrate that our grid-less method is more powerful (it detects sparse alternatives) than tests based on very thin grids.

6.12. Approximate Optimal Designs for Multivariate Polynomial Regression

Y. De Castro, F. Gamboa, D. Henrion, R. Hess, J.-B Lasserre

In [19], 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.

6.13. Simulation of multiphase porous media flows with minimizing movement and finite volume schemes

C .Cancès, T. O. Gallouët, M. Laborde, L. Monsaingeon

In [17]: the Wasserstein gradient flow structure of the PDE system governing multiphase flows in porous media was recently highlighted in [85]. The model can thus be approximated by means of the minimizing movement (or JKO) scheme. We solve the JKO scheme using the ALG2-JKO scheme proposed in [55]. The numerical results are compared to a classical upstream mobility Finite Volume scheme, for which strong stability properties can be established.

6.14. An unbalanced optimal transport splitting scheme for general advection-reaction-diffusion problems

T. O. Gallouët, M. Laborde, L. Monsaingeon

In [21] the authors show that unbalanced optimal transport provides a convenient framework to handle reaction and diffusion processes in a unified metric framework. We use a constructive method, alternating minimizing movements for the Wasserstein distance and for the Fisher-Rao distance, and prove existence of weak solutions for general scalar reaction-diffusion-advection equations. We extend the approach to systems of multiple interacting species, and also consider an application to a very degenerate diffusion problem involving a Gamma-limit. Moreover, some numerical simulations are included.

6.15. Generalized compressible fluid flows and solutions of the Camassa-Holm variational model

T. O. Gallouët, A. Natale, F-X. Vialard

In [35] : The Camassa-Holm equation on a domain M $\in \mathbb{R}^d$, in one of its possible multi-dimensional generalizations, describes geodesics on the group of diffeomorphisms with respect to the H(div) metric. It has been recently reformulated as a geodesic equation for the L2 metric on a subgroup of the diffeomorphism group of the cone over M. We use such an interpretation to construct an analogue of Brenier's generalized incompressible Euler flows for the Camassa-Holm equation. This involves describing the fluid motion using probability measures on the space of paths on the cone, so that particles are allowed to split and cross. Differently from Brenier's model, however, we are also able to account for compressibility by employing an explicit probabilistic representation of the Jacobian of the flow map. We formulate the boundary value problem associated to the Camassa-Holm equation using such generalized flows. We prove existence of solutions and that, for short times, smooth solutions of the Camassa-Holm equations are the unique solutions of our model. We propose a numerical scheme to construct generalized solutions on the cone and present some numerical results illustrating the relation between the generalized Camassa-Holm and incompressible Euler solutions.

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

T. O. Gallouët, F-X. Vialard

In [23]: The group of diffeomorphisms of a compact manifold endowed with the L^2 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 L^2-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 L^2 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 S_1, solutions to the standard CH thus give particular solutions of the incompressible Euler equation on a group of homeomorphisms of $\mathbb{R}^2$ 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.

6.17. Variational Second-Order Interpolation on the Group of Diffeomorphisms with a Right-Invariant Metric

F-X. Vialard

In [38] we propose a variational framework in which the minimization of the acceleration on the group of diffeomorphisms endowed with a right-invariant metric is well-posed. It relies on constraining the acceleration to belong to a Sobolev space of higher-order than the order of the metric in order to gain compactness. It provides the theoretical guarantee of existence of minimizers which is compulsory for numerical simulations.

6.18. Interpolating between Optimal Transport and MMD using Sinkhorn Divergences

J. Feydy, T. Séjourné, F.X. Vialard, S-I. Amari, A. Trouvé, G. Peyré

In [33]: Comparing probability distributions is a fundamental problem in data sciences. Simple norms and divergences such as the total variation and the relative entropy only compare densities in a point-wise manner and fail to capture the geometric nature of the problem. In sharp contrast, Maximum Mean Discrepancies (MMD) and Optimal Transport distances (OT) are two classes of distances between measures that take into account the geometry of the underlying space and metrize the convergence in law. This paper studies the Sinkhorn divergences, a family of geometric divergences that interpolates between MMD and OT. Relying on a new notion of geometric entropy, we provide theoretical guarantees for these divergences: positivity, convexity and metrization of the convergence in law. On the practical side, we detail a numerical scheme that enables the large scale application of these divergences for machine learning: on the GPU, gradients of the Sinkhorn loss can be computed for batches of a million samples.

NACHOS Project-Team

6. New Results

6.1. Electromagnetic wave propagation

6.1.1. POD-based reduced-order DGTD method

Participants: Stéphane Lanteri, Kun Li [UESTC, Chengdu, China], Liang Li [UESTC, Chengdu, China].

This study is concerned with reduced-order modeling for time-domain electromagnetics and nanophotonics. More precisely, we consider the applicability of the proper orthogonal decomposition (POD) technique for the system of 3D time-domain Maxwell equations, possibly coupled to a Drude dispersion model, which is employed to describe the interaction of light with nanometer scale metallic structures. We introduce a discontinuous Galerkin (DG) approach for the discretization of the problem in space based on an unstructured tetrahedral mesh. A reduced subspace with a significantly smaller dimension is constructed by a set of POD basis vectors extracted offline from snapshots that are obtained by the global DGTD scheme with a second order leap-frog method for time integration at a number of time levels. POD-based ROM is established by projecting (Galerkin projection) the global semi-discrete DG scheme onto the low-dimensional space. The stability of the POD-based ROM equipped with the second order leap-frog time scheme has been analysed through an energy method. Numerical experiments have allowed to verify the accuracy, and demonstrate the capabilities of the POD-based ROM. These very promising preliminary results are currently consolidated by assessing the efficiency of the proposed POD-based ROM when applied to the simulation of 3D nanophotonic problems.

6.1.2. Numerical treatment of non-local dispersion for nanoplasmonics

Participants: Herbert de Gersem [TEMF, Technische Universität Darmstadt, Germany], Stéphane Lanteri, Antoine Moreau [Université Clermont Auvergne], Claire Scheid, Dimitrios Loukrezis [TEMF, Technische Universität Darmstadt, Germany], Serge Nicaise [Université de Valenciennes et du Hainaut-Cambresis], Armel Pitelet [Université Clermont Auvergne], 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 (called plasmons) can be excited and cause extreme local field enhancements. 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 response due to electron collisions have to be taken into account. This leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. The classical model is based on a hydrodynamical approach that takes non-local response of the electrons into account. We in particular focus our attention on the linearized version of this model called Linearized Hydrodynamical Drude model. We conducted numerical studies in 2D (published in 2016) and 3D on a linearized hydrodynamic model (published in 2018). However differences between local and nonlocal response are still small. Especially for today's fabrication precision, it remains a challenging task to find reliable structures where non-locality is dominant over e.g. geometrical errors. Motivated by trying to find experimental setups where non-locality is clearly distinguishable from other effects, we studied two promising structures, in close collaboration with physicists. First, in collaboration with A. Pitelet and A. Moreau from Université Clermont Auvergne, and D. Loukrezis and H. De Gersem from Technische Universität Darmstadt, we studied the impact of non-locality on gratings and showed that non-locality can affect surface plasmons

propagating at the interface between a metal and a dielectric with a sufficiently high permittivity. We then design a grating coupler that should allow to experimentally observe this influence. Finally, we carefully set up a procedure to measure the signature of spatial dispersion precisely, paving the way for future experiments. Indeed, to ensure that the impact of non-locality exceeds geometric fabrication uncertainties, we proposed a post-fabrication characterization of the grating coupler. Based on the solution of inverse problems leading to the actually fabricated geometry and an uncertainty quantification (UQ) analysis, we conclude that non-locality should clearly be measurable in the grating coupler setting. This work has been submitted in a physics journal. Secondly in collaboration with A. Moreau we considered a nanocube setup that consists of an infinite gold ground layer plus a dielectric spacer of a given height above which a silver nanocube is chemically deposited. Due to this particular setting, the illumination of such a device is creating inside the gap between the nanocube and the ground layer (i.e. inside the dielectric layer) a gap plasmon that is very sensitive to non-locality. We proposed a surrogate-model based telemetry strategy in order to obtain the fabricated cube dimension (inverse problem). Based on this geometric characterization, we decreased the gap-size between the gold substrate and the silver cube and have compared local and non-local numerical simulations. We showed that the influence of non-locality exceeds the experimental error-bars for gap-sizes below 3.1 nm. Additionally, our nonlocal simulations are able to explain the discrepancy between the experiment and local simulations for very small gap-sizes. This project is still ongoing, since we are waiting for another set of experimental results.

On a theoretical side, we pursue the collaboration with S. Nicaise (Université de Valenciennes et du Hainaut-Cambresis) and proved well-posedness of the linearized non-local Drude model for various boundary conditions. We furthermore focused on establishing polynomial stability with optimal energy decay rate. We conducted a thorough study of energy stability for various numerical schemes and DG formulation using a general framework and finally numerically investigate the discrete polynomial stability. This work is almost finalized.

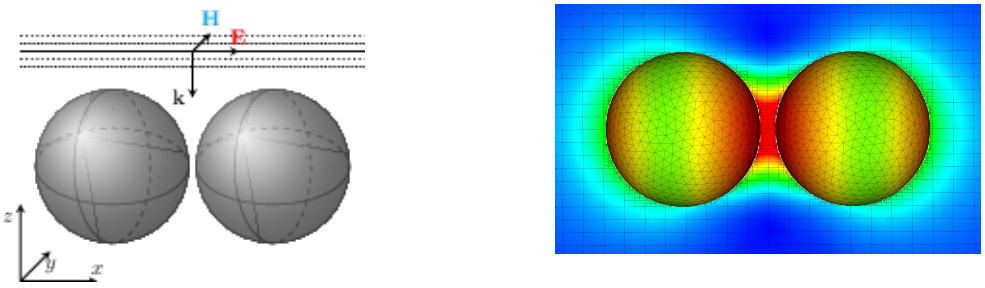


Figure 4. Nanosphere dimer system. Left figure sketches the dimer setup with an $\mathbf{e}_x$ polarized incident plane wave. Right figure shows the 3D field distribution of the electric field on the dimer surface and on a cutting plane and along the dimer axis (PhD thesis of Nikolai Schmitt).

6.1.3. Study of 3D periodic structures at oblique incidences

Participants: Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.

In this work, we focus on the development of the use of periodic boundary conditions with sources at oblique incidence in a DGTD framework. Whereas in the context of the Finite Difference Time Domain (FDTD) methods, an abundant literature can be found, for DGTD, the amount of contributions reporting on such methods is remarkably low. In this work, we supplement the existing references using the field transform technique with an analysis of the continuous system using the method of characteristics and provide an energy estimate. Furthermore, we also study the numerical stability of the resulting DGTD scheme. After numerical validations, two realistic test problems have been considered in the context of nanophotonics with our DIOGENeS DGTD solver. This work is under review.

6.1.4. Toward thermoplasmonics

Participants: Yves d'Angelo, Guillaume Baffou [Fresnel Institute, Marseille], Stéphane Lanteri, Claire Scheid.

Although losses in metal is viewed as a serious drawback in many plasmonics experiments, thermoplasmonics is the field of physics that tries to take advantage of the latter. Indeed, the strong field enhancement obtained in nanometallic structures lead to a localized raise of the temperature in its vicinity leading to interesting photothermal effects. Therefore, metallic nanoparticles may be used as heat sources that can be easily integrated in various environments. This is especially appealing in the field of nanomedecine and can for example be used for diagnosis purposes or nanosurgery to cite but just a few. This year, we initiated a preliminary work towards this new field in collaboration with Y. D'Angelo (Université Côte d'Azur) and G. Baffou (Fresnel Institute, Marseille) who is an expert in this field. Due to the various scales and phenomena that come into play, the numerical modeling present great challenges. The laser illumination first excite a plasmon oscillation (reaction of the electrons of the metal) that relaxes in a thermal equilibrium and in turn excite the metal lattice (phonons). The latter is then responsible for heating the environment. A relevant modeling approach thus consists in describing the electron-phonon coupling through the evolution of their respective temperature. Maxwell's equations is then coupled to a set of coupled nonlinear hyperbolic equations describing the evolution of the temperatures of electrons, phonons and environment. The nonlinearities and the different time scales at which each thermalization occurs make the numerical approximation of these equations quite challenging.

6.1.4.1. Numerical modeling of metasurfaces

Participants: Loula Fezoui, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], 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.

6.1.4.2. 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/triangular 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.

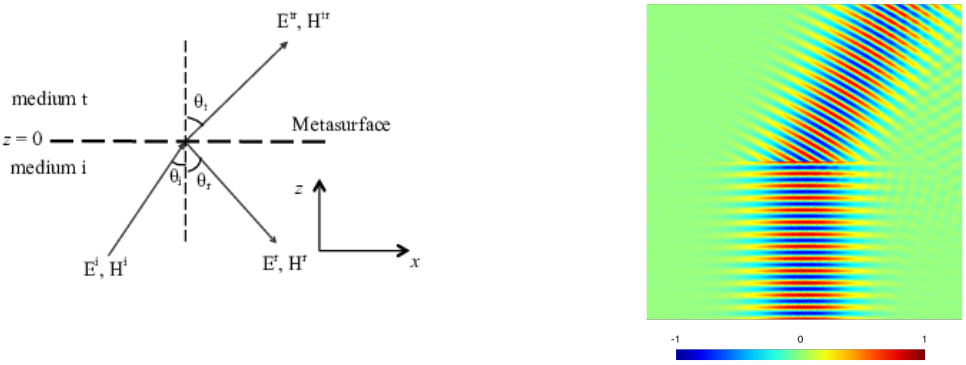


Figure 5. Simulation of a generalized refracting metasurface: problem formulation (left) and real part of H_y, refraction at $\theta = \pi/6$ (right).

6.1.4.3. MHM methods for the time-domain Maxwell equations

Participants: Alexis Gobé, Stéphane Lanteri, 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.

6.1.4.4. MHM methods for the frequency-domain Maxwell equations

Participants: Théophile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri, Frédéric Valentin [LNCC, Petropolis, Brazil].

We have initiated this year a study of MHM methods for the system of frequency-domain Maxwell equations based on very promising results recently obtained by T. Chaumont-Frelet and F. Valentin for the Helmholtz equation. The design principles are very similar to those underlying MHM methods for the system of time-domain Maxwell equations however we expect to achieve more convincing results for highly multiscale problems since we do not have to deal with the time dimension in the present case. Part of this study is conducted in the context of the PHOTOM (PHOTOvoltaic solar devices in Multiscale computational simulations) Math-Amsud project.

6.1.4.5. HDG methods for the time-domain Maxwell equations

Participants: Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.

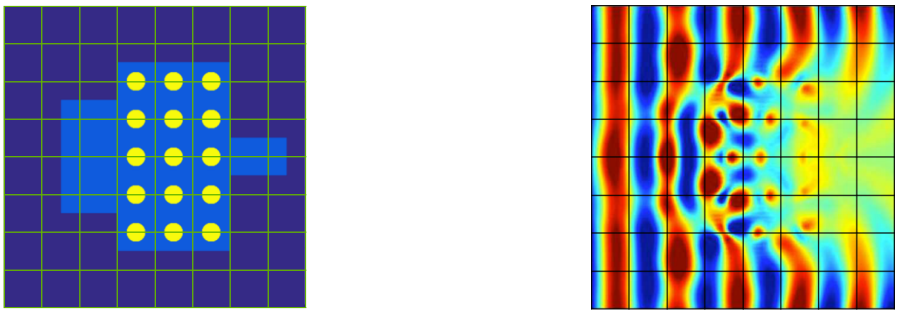


Figure 6. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

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 studied the stability of this new HDG method and in particular, the influence of the stabilization parameter on the CFL condition. We are now progressing toward the design of a new family of high order in time hybrid explicit-implicit HDG methods to deal efficiently with CFL restriction due to grid-induced stiffness.

6.1.4.6. HDG methods for frequency-domain plasmonics

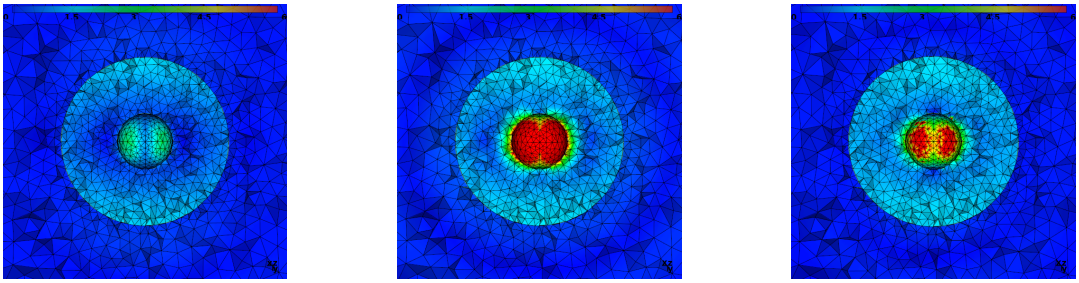
Participants: Stéphane Lanteri, Mostafa Javadzadeh Moghtader, Liang Li [UESTC, Chengdu, China].

HDG method is a new class of DG family with significantly less globally coupled unknowns, and can leverage a post-processing step to gain super-convergence. Its features make HDG a possible candidate for computational electromagnetics applications, especially in the frequency-domain. The HDG method introduces an hybrid variable, which represents an additional unknown on each face of the mesh, and leads to a sparse linear system in terms of the degrees of freedom of the hybrid variable only. Our HDG method had been first introduced for the system of 3D time-harmonic Maxwell's, combined to an iterative Schwarz domain decomposition (DD) algorithm to allow for an efficient parallel hybrid iterative-direct solver. The resulting DD-HDG solver has been applied to classical applications of electromagnetics in the microwave regime. In the present study we further focus on this particular physical context and propose a arbitrary high order HDG method for solving the system of 3D frequency-domain Maxwell equations coupled to a generalized model of physical dispersion in metallic nanostructures at optical frequencies. Such a generalized dispersion model unifies most common dispersion models, like Drude and Drude-Lorentz models, and it permits to fit large range of experimental data. The resulting DD-HDG solver is capable of using different element types and orders of approximation, hence enabling the possibilities of p-adaptivity and non-conforming meshing, and proves to have interesting potentials for modeling of complex nanophotonic and nanoplasmonic problems.

6.2. Elastodynamic wave propagation

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

Participants: Marie-Hélène Lallemand, Claire Scheid, Weslley Da Silva Pereira [LNCC, Petropolis, Brazil], Frédéric Valentin [LNCC, Petropolis, Brazil].



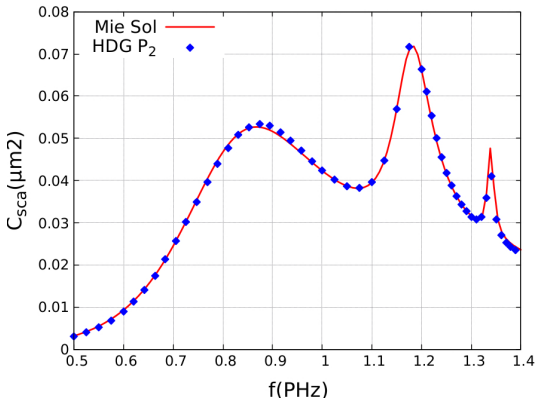


Figure 7. Top figures: scattering of a plane wave by a 50 nm gold nanosphere: magnitude of $\mathbf{E}$ *field at frequencies 1070 THz (left), 1185 THz (middle) and 1300 THz (right). Simulations based on a HDG-*$\mathbb{P}_2$ *method. Bottom figure: Scattering cross section.*

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

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Cristobal Samaniego Alvarado [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Mathieu Faverge [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, Grégoire Pichon [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Pierre Ramet [HIEPACS project-team, Inria Bordeaux - Sud-Ouest].

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at 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 collaborate with the HIEPACS project-team at Inria Bordeaux - Sud-Ouest in view of adapting and exploiting the MaPHyS (Massively Parallel Hybrid Solver - https://gitlab.inria.fr/solverstack/maphys) algebraic hybrid iterative-direct domain decomposition solver. More precisely, this collaboration is concerned with two topics: one one hand, the improvement of the iterative convergence of MaPHyS for the HDG hybrid variable linear system and, on the other hand, the leveraging of low rank compression techniques for reducing the memory footprint of the factorization of subdomain problems using the PaStiX (Parallel Sparse matriX package - http://pastix.gforge.inria.fr/) package.

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

Participants: Stéphane Lanteri, Laércio Lima Pilla [CORSE project-team, Inria Grenoble - Rhône Alpes], Jean-François Méhaut [CORSE project-team, Inria Grenoble - Rhône Alpes].

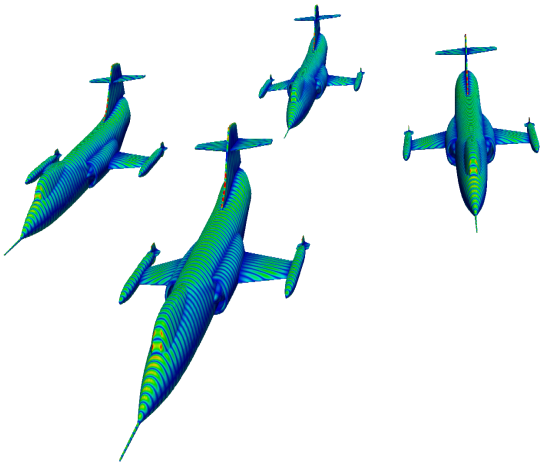


Figure 8. Scattering of a plane wave by a squadron Lockheed F-104 Starfighter. Contour lines of the amplitude of **E** *field. Simulations are performed with a HDG scheme based on a cubic interpolation of the electric and magnetic field unknowns, combined with a PDE-based domain decomposition solver.*

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at the development of a hybrid MPI/OpenMP parallellization of the DGTD solver of the DIOGENeS software suite. In practice, we concentrated our efforts on identifying and evaluating the best approaches for implementing fine grain parallism of the main DG numerical kernels, based on OpenMP features for loop-based parallelism on one hand, and task-based parallelism on the other hand.

6.4. Applications

6.4.1. 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.

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).

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.

6.4.2. Photovoltaics

The ultimate success of photovoltaic (PV) cell technology requires substantial progress in both cost reduction and efficiency improvement. An actively studied approach to simultaneously achieve these two objectives is to leverage *light trapping* schemes. Light trapping allows solar cells to absorb sunlight using an active material layer that is much thinner than the material's intrinsic absorption length. This then reduces the amount of materials used in PV cells, which cuts cell cost in general, and moreover facilitates mass production of PV cells that are based on less abundant materials. In addition, light trapping can improve cell efficiency, since thinner cells provide better collection of photo-generated charge carriers. Enhancing the light absorption in ultrathin film silicon solar cells is thus of paramount importance for improving efficiency and reducing cost. We are involved in several studies in collaboration with physicists that aim at simulating light trapping in complex solar cell structures using high order DG and HDG solvers developed in our core research activities.

6.4.2.1. Light-trapping in texturized thin film 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.

6.4.2.2. Light-trapping in nanocone gratings

Participants: Stéphane Collin [Sunlit team, C2N-CNRS, Marcoussi], Alexis Gobé, Julie Goffard [Sunlit team, C2N-CNRS, Marcoussi], Stéphane Lanteri.

There is significant recent interest in designing ultrathin crystalline silicon solar cells with active layer thickness of a few micrometers. Efficient light absorption in such thin films requires both broadband antireflection coatings and effective light trapping techniques, which often have different design considerations. In collaboration with physicists from the Sunlit team at C2N-CNRS, we conduct a numerical study of solar cells based on nanocone gratings. Indeed, it has been previously shown that by employing a double-sided grating design, one can separately optimize the geometries for antireflection and light trapping purposes to achieve broadband light absorption enhancement [47]. In the present study, we adopt the nanocone grating considered in [47]. This structure contains a crystalline silicon thin film with nanocone gratings also made of silicon. The circular

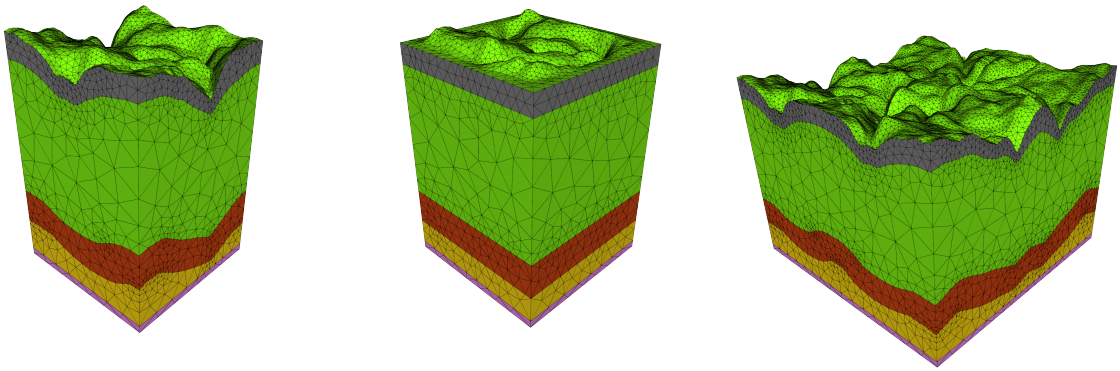


Figure 10. Simulation of light trapping in a multi-layer solar cell with surface texture using a high order DGTD fullwave solver and topography conforming geometrical models.

nanocones form two-dimensional square lattices on both the front and the back surfaces. The film is placed on a perfect electric conductor (PEC) mirror. The ultimate objective of this study is to devise a numerical optimization strategy to infer optimal values of the geometrical characteristics of the nanocone grating on each side of the crystalline silicon thin film. Absorption characteristics are here evaluated using the high order DGTD solver from the DIOGENeS software suite.

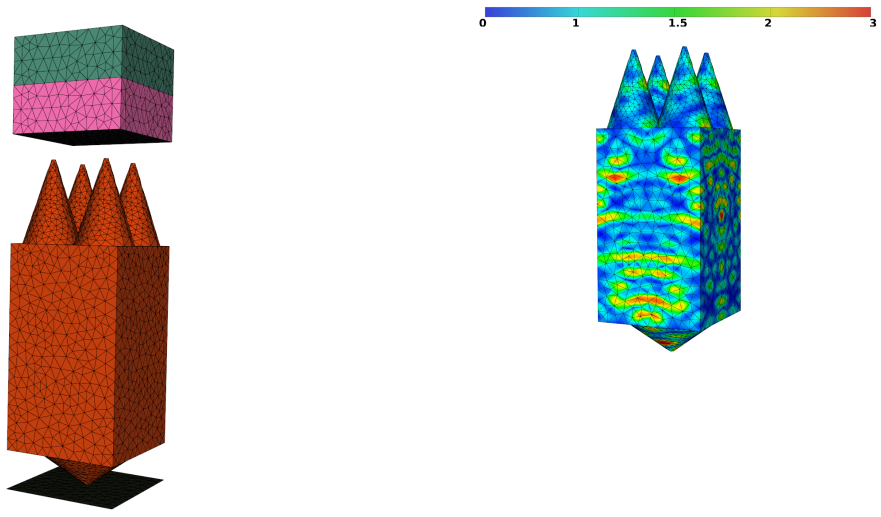


Figure 11. Simulation of light trapping in a solar cell based on nanocone gratings. Geometrical model (left) and contour lines of the module of the DFT of $\mathbf{E}$ *for a wavelength* $\lambda = 857$ *nm (right).*

6.4.3. Inver design of metasurfaces

Participants: Régis Duvigneau [ACUMES project-team, Inria Sophia Antipolis-Méditerranée], Mahmoud Elsawy, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Stéphane Lanteri.

Metasurfaces are flat surfaces consisting of sub-wavelength nanoresonators, made of plasmonic or high dielectric refractive index materials patterned in a specific way. These flat surfaces provide nearly full control of the light properties in a very short propagation distance with high resolution. By changing the dimensions, shapes, and orientation of these nanoresonators, different functionalities can be obtained. The complexity of the problem and the wide parameter space, make the direct modelling problem insufficient. Recently, several optimization techniques have been applied to the field of nanophotonics (including metasurfaces) by solving an inverse design problem. Generally speaking, there are two classes of optimization techniques that have been used in the metasurface designs; local and global techniques. The local methods depend on the initial guess and most of them require the computation of the gradient, which might be challenging. In addition, they are limited to small parameter space. On the other hand, global optimization techniques are suitable for optimizing several parameters moreover, they do not stuck in a local minima/maxima like the local methods. However, most of the global techniques used in the metasurface designs require costly simulations (for large parameter space), which make them inapplicable for modeling real-life designs that require 3D fullwave solvers. In this study conducted in collaboration with physicists at CRHEA, we use two efficient global optimization techniques based on statistical learning in order to overcome the disadvantageous of usual global optimization methods. The first one is the covariance matrix adaptation evolutionary strategy (CMA-ES). The CMA-ES has been gaining a lot of attention since it requires fewer cost function evaluations compared to the other evolutionary algorithms like genetic algorithms especially for 3D problems that require expensive simulations even with the high-performance computational resources. The second method is the Efficient Global Optimization (EGO) algorithm. The EGO algorithm is based on the surrogate modelling, that is to say, replacing the complex or costly evaluation process by a simpler and cheaper model to reduce dramatically the computational cost (number of calls for the electromagnetic simulations). Both techniques are offered by the Famosa library (http://famosa.gforge.inria.fr), which is developed by R. Duvigneau and colleagues in the ACUMES project-team.

NANO-D Project-Team

6. New Results

6.1. Generating conformational transition paths with low potential-energy barriers for proteins

Participants: Minh Khoa Nguyen, Léonard Jaillet and Stéphane Redon.
Publication: Journal of Computer-Aided Molecular Design, 2018 [66].

The knowledge of conformational transition paths in proteins can be useful for understanding protein mechanisms. Recently, we have introduced the As-Rigid-As-Possible (ARAP) interpolation method, for generating interpolation paths between two protein conformations. The method was shown to preserve well the rigidity of the initial conformation along the path. However, because the method is totally geometry-based, the generated paths may be inconsistent because the atom interactions are ignored. Therefore, we introduce a new method to generate conformational transition paths with low potential-energy barriers for proteins. The method is composed of three processing stages. First, ARAP interpolation is used for generating an initial path. Then, the path conformations are enhanced by a clash remover. Finally, Nudged Elastic Band, a path-optimization method, is used to produce a low-energy path. Large energy reductions are found in the paths obtained from the method than in those obtained from the ARAP interpolation method alone. The results also show that ARAP interpolation is a good candidate for generating an initial path because it leads to lower potential-energy paths than two other common methods for path interpolation (see Figure 1 for an example of optimized transition path).

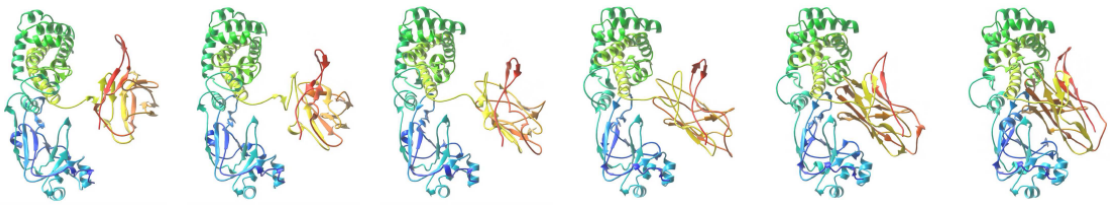


Figure 1. The path for diphtheria toxin after ARAP interpolation and NEB optimization.

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

Participants: Minh Khoa Nguyen, Leonard Jaillet, Stephane Redon.
Publication: Journal of Computational Chemistry, 2018 [65].

We have proposes a method to efficiently generate approximate ligand unbinding pathways. 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 (see Figure 2).

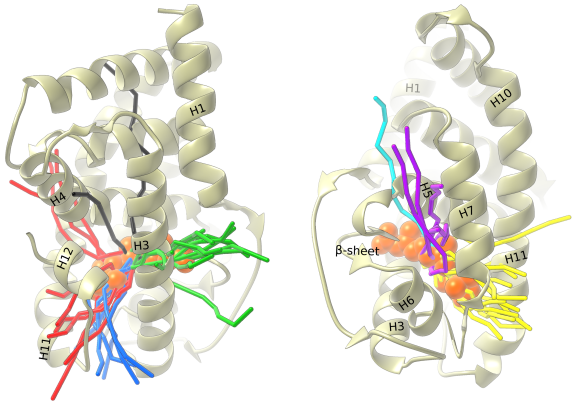


Figure 2. Families of paths (in colored sticks) obtained with ART-RRT for the unbinding of retinoic acid hormone from its receptor. The protein is represented by ribbons and the ligand by orange balls.

6.3. Atomistic modelling and simulation of transmission electron microscopy images: application to intrinsic defects of graphene

Participants: Cyril Guedj, Léonard Jaillet, François Rousse and Stéphane Redon.
Publication: Proceedings of 8th International Conference on Simulation and Modeling Methodologies, Technologies and Applications - Volume 1: SIMULTECH [53].
The characterization of advanced materials and devices in the nanometer range requires complex tools, and the data analysis at the atomic level is required to understand the precise links between structure and properties. We have demonstrated that the atomic-scale modelling of graphene-based defects may be performed efficiently for various structural arrangements using the Brenner module of the SAMSON software platform (cf Figure 3). The signatures of all kinds of defects are computed in terms of energy and scanning transmission electron microscopy simulated images. The results are in good agreement with all theoretical and experimental data available. This original methodology is an excellent compromise between the speed and the precision required by the semiconductor industry and opens the possibility of realistic in-silico research conjugated to experimental nanocharacterisation of these promising materials.

6.4. Impact of hydrogen on graphene-based materials: atomistic modeling and simulation of HRSTEM images.

Participants: Cyril Guedj, Léonard Jaillet, François Rousse and Stéphane Redon.
Oral presentation: AVS 65th International Symposium and Exhibition.
Summary: The hydrogen energy transition is highly probable, because hydrogen is the most abundant element in the universe and represents an ideal “green” source of energy. Meanwhile, the safe hydrogen production and storage remains a major challenge still in progress. To understand and optimize the device efficiency and the interface engineering, it is advantageous to perform advanced nanocharacterizations, linked to numerical modelling and simulations. This task is particularly difficult, because hydrogen is labile and prone to rapid reorganization. This structural evolution may be monitored with transmission electron microscopy (TEM) techniques, but in spite of significant progresses, the direct detection of hydrogen with High Resolution Scanning Transmission Electron Microscopy (HRSTEM) or energy-loss spectroscopy still remains a serious challenge.

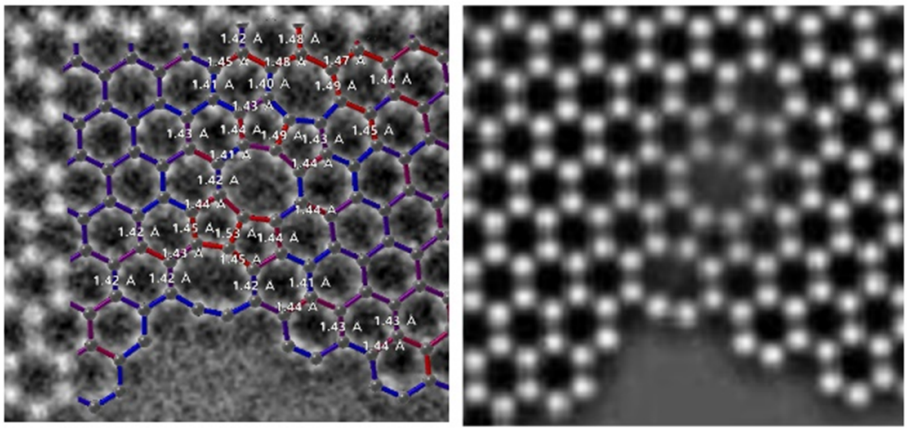


Figure 3. Left: atomistic model of the extended defect 88-7-5555 defect superimposed to the experimental HRTEM image entitled "SALVE-III-project-HRTEM-graphene-vacancy-characteristic-defects.png" (Salve, 2018). Right: corresponding simulated HRTEM image.

We investigate here the interaction of hydrogen with graphene using the Brenner module of the SAMSON software platform and we propose an original methodology to characterize its structural arrangement at the atomic scale by simulating HRSTEM images to interpret experimental results. In particular, we compare the effect of hydrogen on dark field (DF), bright field (BF), high-angle annular dark filed (HAADF) and annular bright field (ABF) images, to estimate the best technique suited to hydrogen detection. In addition, we present the effect of carbon vacancies and adatoms on the stability of hydrogen coverage, associated to the HRSTEM signatures of the most stable configurations. These results provide the necessary building blocks to analyze the structure and energetics of hydrogenated graphene-based materials at the atomic scale.

6.5. Atomistic modelling of diamond-type $Si_xGe_yC_zSn_{1-x-y-z}$ crystals for realistic transmission electron microscopy image simulations

Participants: Leonard Jaillet and Cyril Guedj.
The realistic simulations of transmission electron microscopy (TEM) images requires an accurate definition of the positions of all atoms, which are linked to the mechanical properties of the material. We are working on an approach to build optimized models to represent the lattice parameters and elastic properties of Si, Ge, diamond, alpha-tin and related diamond alloys.

In order to compute precisely the complex $Si_xGe_yC_zSn_{1-x-y-z}$ diamond crystals, a dedicated parametrization of the Keating force field has been proposed. An original periodic boundary strategy has also been provided. Our tool can be used to interpret experimental TEM with a speed several orders of magnitude higher than for ab-initio methods. The method predicts the correct lattice parameters and elastic constants for published experimental results with low deviation. Finally, we have shown that subsequent Monte Carlo simulations predict original self-ordering effects in C in good agreement with the theory. A publication is in preparation on this topic.

6.6. Analytical symmetry detection method AnAnaS

Participants: Guillaume Pagès, Sergei Grudinin, Elvira Kinzina.
Publications: Journal of Structural Biology, 2018 [21], Journal of Structural Biology, 2018 [20].

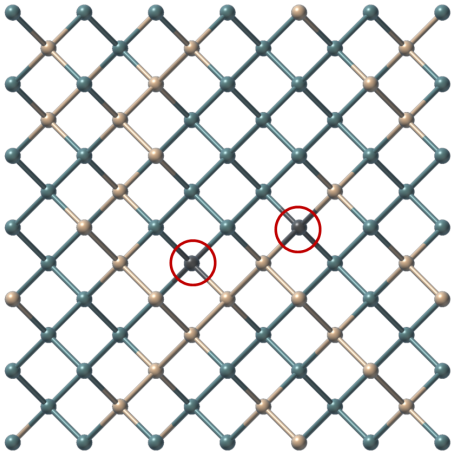


Figure 4. Crystal of $Si_{40}Ge_{60}$ where two carbon atoms (circled in red) have been inserted. The properties of the crystal such as its lattice parameter can be characterized in function of the position of the carbon atoms.

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 papers describing the method were published [21], [20]. This method is available on the website of the team (https://team.inria.fr/nano-d/software/ananas/).

6.7. Deep Learning for Symmetry detection

Participants: Guillaume Pagès, Sergei Grudinin.
Publication: arXiv preprint, 2018 [29].

We worked on a fully-structural method for detecting symmetries in molecular structures. This allowed 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 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°. A manuscript describing this method has been submitted for publication and is available on arXiv [29].

6.8. New method for protein model quality assessment Ornate

Participants: Benoit Charmettant, Guillaume Pagès, Sergei Grudinin.
Publication: bioRxiv preprint, 2018 [28].

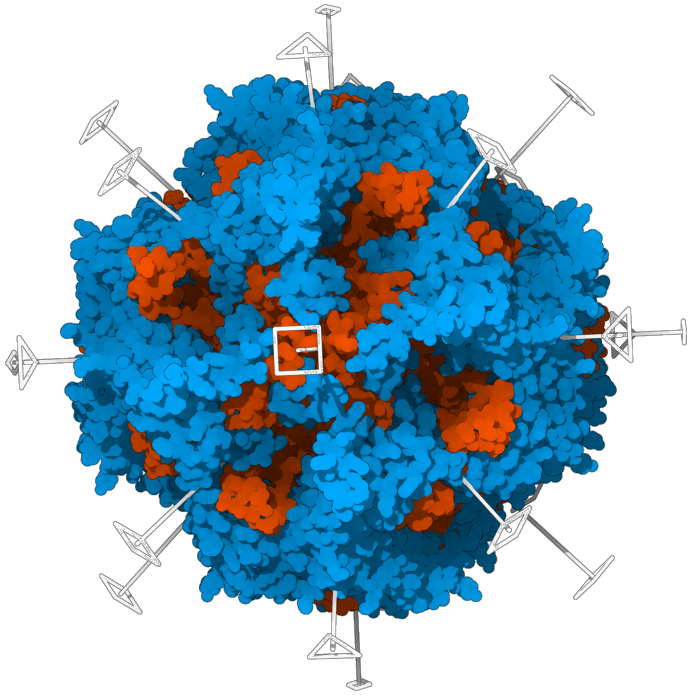


Figure 5. System with an octahedral symmetry, with the symmetry axes displayed in SAMSON.

Protein model quality assessment (QA) is a crucial and yet open problem in structural bioinformatics. It consists of estimating a score to assess whether a given three-dimensional structure is correctly folded or not. The current best methods for single-model QA typically combine results from different approaches, each based on different input features constructed by experts in the field. Then, the prediction model is trained using a machine-learning algorithm. Recently, with the development of convolutional neural networks (CNN), the training paradigm has changed. In computer vision, the expert-developed features have been significantly overpassed by automatically trained convolutional filters. This motivated us to apply a three-dimensional (3D) CNN to the problem of protein model QA.

We developed a novel method for single-model QA called Ornate. Ornate (Oriented Routed Neural network with Automatic Typing) is a residue-wise scoring function that takes as input 3D density maps. It predicts the local (residue-wise) and the global model quality through a deep 3D CNN. Specifically, Ornate aligns the input density map, corresponding to each residue and its neighborhood, with the backbone topology of this residue. This circumvents the problem of ambiguous orientations of the initial models. Also, Ornate includes automatic identification of atom types and dynamic routing of the data in the network. Established benchmarks (CASP 11 and CASP 12) demonstrate the state-of-the-art performance of our approach among single-model QA methods. A manuscript describing this method has been submitted for publication and is available on bioRxiv [28].

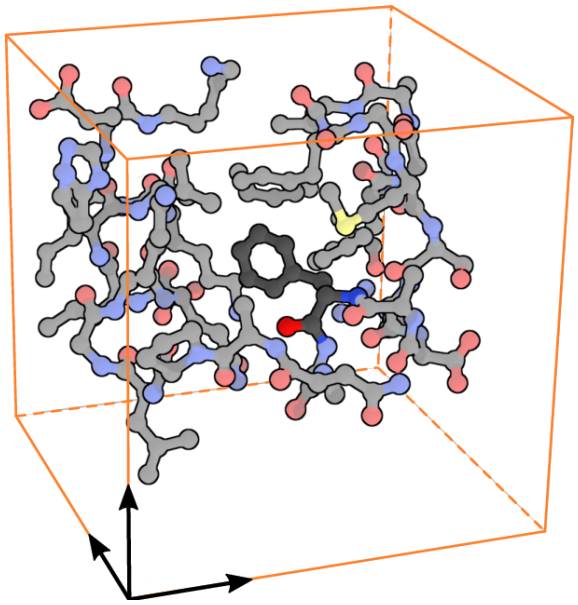


Figure 6. Example of input given to the 3D CNN Ornate.

RAPSODI Project-Team

7. New Results

7.1. Numerical simulation of concrete carbonation

In [20], C. Chainais-Hillairet, B. Merlet, and A. Zurek introduce and study a Finite Volume scheme for a concrete carbonation model proposed by Aiki and Muntean in [50]. 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.

In [45], A. Zurek studies the long-time regime of the moving interface appearing in the concrete carbonation model. He proves that the approximate free boundary, given by an implicit-in-time Finite Volume scheme, increases in time following a $\sqrt{t}$-law. This result is illustrated by numerical experiments.

7.2. Modeling and numerical simulation of complex fluids

In the context of C. Colin-Lecerf's PhD, C. Calgaro Zotto, C. Colin-Lecerf, and E. Creusé derive in [35] a combined Finite Volume-Finite Element scheme for a low-Mach model, in which a temperature field obeying an energy law is taken into account. The continuity equation is solved, whereas the state equation linking temperature, density, and thermodynamic pressure is imposed implicitly. Since the velocity field is not divergence-free, the projection method solving the momentum equation has to be adapted. This combined scheme preserves some steady states, and ensures a discrete maximum principle on the density. Numerical results are provided and compared to other approaches using purely Finite Element schemes, on a benchmark consisting in particular in a transient injection flow [58], [89], [53], as well as in the natural convection of a flow in a cavity [97], [93], [89], [53].

The theoretical study of the low-Mach limit system is a vast subject that has been considered by many authors. In particular, in [86], Embid establishes the local-in-time existence of classical solutions in Sobolev spaces. In [77], Danchin and Liao study the well-posedness issue in the critical Besov spaces, locally and globally, assuming that the initial density is close to a constant and that the initial velocity is small enough. Levermore *et al.* [98] consider the so-called ghost effect system, which is quite similar to the low-Mach system with thermal stress term added to the right-hand-side of the momentum equation, and they prove the local well-posedness of classical solutions for the Cauchy problem. In [94], Huang and Tan prove a local well-posedness result for strong solutions and also the existence and uniqueness of a global strong solution for the two-dimensional case. In [14], C. Calgaro Zotto, C. Colin-Lecerf, E. Creusé *et al.* investigate a specific low-Mach model for which the dynamic viscosity of the fluid is a specific function of the density. The model is reformulated in terms of the temperature and velocity, with nonlinear temperature equation, and strong solutions are considered. In addition to a local-in-time existence result for strong solutions, some convergence rates of the error between the approximation and the exact solution are obtained, following the same approach as Guillén-González *et al.* [91], [92].

Diffuse interface models, such as the Kazhikhov–Smagulov model, allow to describe some phase transition phenomena. In [15], C. Calgaro Zotto and co-workers investigate theoretically the combined Finite Volume-Finite Element 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 [27], I. Lacroix-Violet *et al.* 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 difficulties 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 [34], I. Lacroix-Violet *et al.* 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 justifying 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. The 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 the analysis, Lacroix-Violet *et al.* show that this augmented formulation helps to define relative entropy estimates for the Euler–Korteweg systems in a simpler way and with less hypotheses compared to recent works [82], [88].

7.3. Stratigraphic modeling and simulation

Stratigraphy is a discipline of physics that aims at predicting the geological composition of the subsoil. In [44], N. Peton, C. Cancès *et al.* propose a new water flow driven forward stratigraphic model with the following particularities. First, the water surface flow is modelled at the continuous level, in opposition to what is currently done in this community. Second, the model incorporates a constraint on the erosion rate. A stable numerical scheme is proposed to simulate the model.

7.4. Numerical simulation in low-frequency electromagnetism

In [24], [28], E. Creusé and co-workers investigate the behavior of some Finite Element error estimators in the context of low-frequency elecromagnetism simulations, to underline the main differences in some practical situations. In addition, a more theoretical contribution is developed in [23], to prove the equivalence of some usual discrete gauge conditions. Once again, their numerical behaviors are compared on some characteristic benchmarks.

7.5. Asymptotic analysis

In [33], C. Cancès and co-workers derive the porous medium equation as the hydrodynamic limit of an interacting particle system which belongs to the family of exclusion processes with nearest neighbor exchanges. The main outcome of this work is to allow regions with vanishing density, where the dynamics turns out to degenerate. The convergence builds on a generalization of the entropy method and on suitable regularization of the dynamics.

In [29], A. Ait Hammou Oulhaj, C. Cancès, C. Chainais-Hillairet *et al.* study analytically and numerically the large time behavior of the solutions to a two-phase extension of the porous medium equation, which models the so-called seawater intrusion problem. They identify the self-similar solutions that correspond to steady states of a rescaled version of the problem. They finally provide numerical illustrations of the stationary states and exhibit numerical convergence rates.

In [13], C. Chainais-Hillairet *et al.* propose a new proof of existence of a solution to the scheme introduced in [63] 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 [63].

In [38], C. Chainais-Hillairet and M. Herda study the large-time behavior of solutions to Finite Volume discretizations of convection-diffusion equations or systems endowed with non-homogeneous Dirichlet and Neumann type boundary conditions. Their results concern various linear and nonlinear models such as Fokker–Planck equations, porous media equations, or drift-diffusion systems for semiconductors. For all of these models, some relative entropy principle is satisfied and implies exponential decay to the stationary state. They show that in the framework of Finite Volume schemes on orthogonal meshes, a large class of two-point monotone fluxes preserve this exponential decay of the discrete solution to the discrete steady state of the scheme.

In [32], M. Herda, T. Rey *et al.* are interested in the asymptotic analysis of a Finite Volume scheme for one-dimensional linear kinetic equations, with either Fokker–Planck or linearized BGK collision operator. Thanks to appropriate uniform estimates, they establish that the proposed scheme is asymptotic-preserving in the diffusive limit. Moreover, they adapt to the discrete framework the hypocoercivity method proposed by [80] to prove the exponential return to equilibrium of the approximate solution. They obtain decay estimates that are uniform in the diffusive limit. Finally, they present an efficient implementation of the proposed numerical schemes, and perform numerous numerical simulations assessing their accuracy and efficiency in capturing the correct asymptotic behaviors of the models.

In [26], M. Herda *et al.* consider various sets of Vlasov–Fokker–Planck equations modeling the dynamics of charged particles in a plasma under the effect of a strong magnetic field. For each of them, in a regime where the strength of the magnetic field is effectively stronger than that of collisions, they first formally derive asymptotically reduced models. In this regime, strong anisotropic phenomena occur; while equilibrium along magnetic field lines is asymptotically reached the asymptotic models capture a nontrivial dynamics in the perpendicular directions. They do check that in any case the obtained asymptotic model defines a well-posed dynamical system and when self-consistent electric fields are neglected they provide a rigorous mathematical justification of the formally derived systems. In this last step they provide a complete control on solutions by developing anisotropic hypocoercive estimates.

7.6. Structure-preserving numerical methods

The design and the analysis of numerical methods preserving at the discrete level the key features of the continuous models is one of the core tasks of the RAPSODI project-team. C. Cancès was invited to write a review paper [16] on energy stable numerical methods for complex porous media flows. The paper addresses three different approaches: monotonicity-based numerical methods like two-point flux approximation Finite Volumes, as well as two methods based on multi-point flow approximation that are either based on upwinding or on positive local dissipation tensors.

Concerning methods based on upwinding, A. Ait Hammou Oulhaj, C. Cancès, and C. Chainais-Hillairet extend in [12] the nonlinear Control Volume Finite Element scheme of [69] to the discretization of Richards equation modeling unsaturated flows in porous media. This strategy is also applied in [30] by A. Ait Hammou Oulhaj and D. Maltese for the simulation of seawater intrusion in the subsoil nearby coastal regions. The scheme proposed in [30] is still convergent if the porous medium is anisotropic, in opposition to the energy-diminishing scheme analyzed in [11] by A. Ait Hammou Oulhaj, which is designed to be accurate in the long-time regime studied in [29]. Besides, an implicit Euler-Finite Volume scheme for a degenerate cross-diffusion system describing the ion transport through biological membranes is analyzed in [17] by C. Cancès, C. Chainais-Hillairet *et al.* The strongly coupled equations for the ion concentrations include drift terms involving the electric potential, which is coupled to the concentrations through the Poisson equation. The cross-diffusion system possesses a formal gradient flow structure revealing nonstandard degeneracies, which lead to considerable mathematical difficulties. The Finite Volume scheme is based on two-point flux approximations with "double" upwind mobilities. It preserves the structure of the continuous model like non-negativity, upper bounds, and entropy dissipation.

Concerning methods based on positive local dissipation tensors, C. Cancès, C. Chainais-Hillairet *et al.* propose in [18] a nonlinear Discrete Duality Finite Volume scheme to approximate the solutions of drift diffusion equations. The scheme is built to preserve at the discrete level even on severely distorted meshes

the energy/energy dissipation relation. In [37], C. Cancès and co-workers propose a Finite Element scheme for the numerical approximation of degenerate parabolic problems in the form of a nonlinear anisotropic Fokker–Planck equation. The scheme is energy-stable, only involves physically motivated quantities in its definition, and is able to handle general unstructured grids. Its convergence is rigorously proven thanks to compactness arguments, under very general assumptions. Although the scheme is based on Lagrange Finite Elements of degree 1, it is locally conservative after a local post-processing giving rise to an equilibrated flux. This also allows to derive a guaranteed *a posteriori* error estimate for the approximate solution. Numerical experiments are presented in order to give evidence of a very good behavior of the proposed scheme in various situations involving strong anisotropy and drift terms.

C. Cancès *et al.* derive in [36] 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 [106], [85]) and is closely related to a model proposed by E and collaborators [84], [100]. Besides the derivation of the model, the convergence of a minimizing movement scheme is proven in [36]. The Wasserstein gradient flow structure of the PDE system governing multiphase flows in porous media has recently been highlighted in [68]. The model can thus be approximated by means of the minimizing movement (or JKO) scheme, that C. Cancès *et al.* solve in [19] thanks to the ALG2-JKO scheme proposed in [60]. The numerical results are compared to a classical upstream mobility Finite Volume scheme, for which strong stability properties can be established.

In [42], S. Lemaire builds a bridge between the Hybrid High-Order [78] and Virtual Element [59] methods, which are the two main new-generation approaches to the arbitrary-order approximation of PDEs on meshes with general, polytopal cells. The Virtual Element method writes in functional terms and is naturally conforming; at the opposite, the Hybrid High-Order method writes in algebraic terms and is naturally nonconforming. It has been remarked a few years ago that the Hybrid High-Order method can be viewed as a nonconforming version of the Virtual Element method. In [42], S. Lemaire ends up unifying the Hybrid High-Order and Virtual Element approaches by showing that the Virtual Element method can be reformulated as a (newborn) conforming Hybrid High-Order method. This parallel has interesting consequences: it allows important simplifications in the *a priori* analysis of Virtual Element methods, and sheds new light on the differences between conforming and nonconforming Virtual Element methods, in particular in terms of mesh assumptions.

In [31], I. Lacroix-Violet *et al.* are interested in the numerical integration in time of nonlinear Schrödinger equations using different methods preserving the energy or a discrete analog of it. In particular, they give a rigorous proof of the order of the relaxation method (presented in [62] for cubic nonlinearities) and they propose a generalized version that allows to deal with general power law nonlinearities. Numerical simulations for different physical models show the efficiency of these methods.

7.7. Cost reduction for numerical methods

In [22], S. Lemaire *et al.* design and analyze (in the periodic setting) nonconforming multiscale methods for highly oscillatory elliptic problems, which are applicable on coarse grids that may feature general polytopal cells. Two types of methods are introduced: a Finite Element-type method, that generalizes classical nonconforming multiscale Finite Element methods to general meshes and to arbitrary-order polynomial cell boundary conditions, and a Virtual Element-type method, that allows, up to the computation of an adequate projection, to compute less oscillatory basis functions for equivalent precision. The Virtual Element-type method is based on the Hybrid High-Order framework [78]. As standard with such multiscale approaches, the general workflow of the method splits into an offline, massively parallelizable stage, where all fine-scale computations are performed, and the online, fully-coarse-scale stage.

In [25], T. Rey *et al.* 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 dynamics.

In [43], T. Rey *et al.* present high-order, fully explicit time integrators for nonlinear collisional kinetic equations, including the full Boltzmann equation. The methods, called projective integration, first take a few small steps with a simple, explicit method (forward Euler) to damp out the stiff components of the solution. Then, the time derivative is estimated and used in a Runge–Kutta method of arbitrary order. The procedure can be recursively repeated on a hierarchy of projective levels to construct telescopic projective integration methods. We illustrate the method with numerical results in one and two spatial dimensions.

7.8. Applied calculus of variations

In [41], B. Merlet *et al.* study a variational problem which models the behavior of topological singularities on the surface of a biological membrane in P_β-phase (see [103]). 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 $\varepsilon > 0$. B. Merlet *et al.* perform a complete Γ-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.

In [21], B. Merlet *et al.* consider a generalization of branched transport in arbitrary dimension and codimension: minimize the h-mass of some oriented k-dimensional branched surface in $\mathbf{R}^n$ with some prescribed boundary. Attached to the surface is a multiplicity $m(x)$ which is not necessarily an integer and is a conserved quantity (Kirchhoff current law is satisfied at branched points). The h-mass is defined as the integral of a cost $h(|m(x)|)$ over the branched surface. As usual in branched transportation, the cost function is a lower-semicontious, sublinear increasing function with $h(0) = 0$ (for instance $h(m) = \sqrt{1 + am^2}$ if $m \neq 0$ and $h(0) = 0$). For numerical purpose, it is convenient to approximate the measure defined by the k-dimensional surfaces by smooth functions in $\mathbf{R}^n$. In this spirit, B. Merlet *et al.* propose phase field approximations of the branched surfaces and of their energy in the spirit of the Ambrosio–Tortorelli functional. The convergence of these approximations towards the original k-dimensional branched transport problem is established in [21] in the sense of Γ-convergence. Next, considering the cost $h(m) = \sqrt{1 + am^2}$ and sending a to 0, a phase field approximation of the Plateau problem is obtained. Numerical experiments show the efficiency of the method. These numerical results are exceptional as they are obtained without any guess on the topology of the minimizing k-surface (as opposed to methods based on parameterizations of the k-surface). In [39], B. Merlet *et al.* establish new results on the approximation of k-dimensional surfaces (k-rectifiable currents) by polyhedral surfaces with convergence in h-mass and with preservation of the boundary (the approximating polyhedral surface has the same boundary as the limit). This approximation result is required in the convergence study of [21].

7.9. Approximation theory

In [40], M. Herda *et al.* propose a new iterative algorithm for the calculation of sum of squares decompositions of polynomials, reformulated as positive interpolation. The method is based on the definition of a dual functional G from values at interpolation points. The domain of G, the boundary of the domain and the behavior of G at infinity are analyzed in details. In the general case, G is closed convex. For univariate polynomials in the context of the Lukacs representation, G is coercive and strictly convex which yields a unique critical point, corresponding to a sum of squares decomposition of G. Various descent algorithms are evoked. Numerical examples are provided, for univariate and bivariate polynomials.

CAGE Project-Team

6. New Results

6.1. Geometry of vision and sub-Riemannian geometry: new results

Let us list here our new results in the geometry of vision axis and, more generally, on hypoelliptic diffusion and sub-Riemannian geometry.

- In [7] we present a new image inpainting algorithm, the Averaging and Hypoelliptic Evolution (AHE) algorithm, inspired by the one presented in [86] and based upon a (semi-discrete) variation of the Citti–Petitot–Sarti model of the primary visual cortex V1. In particular, we focus on reconstructing highly corrupted images (i.e. where more than the 80% of the image is missing).
- In [6] we deal with a severe ill posed problem, namely the reconstruction process of an image during tomography acquisition with (very) few views. We present different methods that we have been investigated during the past decade. They are based on variational analysis.
- [13] is the first paper of a series in which we plan to study spectral asymptotics for sub-Riemannian Laplacians and to extend results that are classical in the Riemannian case concerning Weyl measures, quantum limits, quantum ergodicity, quasi-modes, trace formulae. Even if hypoelliptic operators have been well studied from the point of view of PDEs, global geometrical and dynamical aspects have not been the subject of much attention. As we will see, already in the simplest case, the statements of the results in the sub-Riemannian setting are quite different from those in the Riemannian one. Let us consider a sub-Riemannian (sR) metric on a closed three-dimensional manifold with an oriented contact distribution. There exists a privileged choice of the contact form, with an associated Reeb vector field and a canonical volume form that coincides with the Popp measure. We establish a Quantum Ergodicity (QE) theorem for the eigenfunctions of any associated sR Laplacian under the assumption that the Reeb flow is ergodic. The limit measure is given by the normalized Popp measure.This is the first time that such a result is established for a hypoelliptic operator, whereas the usual Shnirelman theorem yields QE for the Laplace-Beltrami operator on a closed Riemannian manifold with ergodic geodesic flow. To prove our theorem, we first establish a microlocal Weyl law, which allows us to identify the limit measure and to prove the microlocal concentration of the eigenfunctions on the characteristic manifold of the sR Laplacian. Then, we derive a Birkhoff normal form along this characteristic manifold, thus showing that, in some sense, all 3D contact structures are microlocally equivalent. The quantum version of this normal form provides a useful microlocal factorization of the sR Laplacian. Using the normal form, the factorization and the ergodicity assumption, we finally establish a variance estimate, from which QE follows. We also obtain a second result, which is valid without any ergodicity assumption: every Quantum Limit (QL) can be decomposed in a sum of two mutually singular measures: the first measure is supported on the unit cotangent bundle and is invariant under the sR geodesic flow, and the second measure is supported on the characteristic manifold of the sR Laplacian and is invariant under the lift of the Reeb flow. Moreover, we prove that the first measure is zero for most QLs.
- In [22] we study the validity of the Whitney C^1 extension property for horizontal curves in sub-Riemannian manifolds endowed with 1-jets that satisfy a first-order Taylor expansion compatibility condition. We first consider the equiregular case, where we show that the extension property holds true whenever a suitable non-singularity property holds for the input-output maps on the Carnot groups obtained by nilpotent approximation. We then discuss the case of sub-Riemannian manifolds with singular points and we show that all step-2 manifolds satisfy the C^1 extension property. We conclude by showing that the C^1 extension property implies a Lusin-like approximation theorem for horizontal curves on sub-Riemannian manifolds.

- In [34] we prove the C^1 regularity for a class of abnormal length-minimizers in rank 2 sub-Riemannian structures. As a consequence of our result, all length-minimizers for rank 2 sub-Riemannian structures of step up to 4 are of class C^1.
- In [45] we address the double bubble problem for the anisotropic Grushin perimeter P_α, $\alpha \geq 0$, and the Lebesgue measure in $\mathbb{R}^2$, in the case of two equal volumes. We assume that the contact interface between the bubbles lays on either the vertical or the horizontal axis. Since no regularity theory is available in this setting, in both cases we first prove existence of minimizers via the direct method by symmetrization arguments and then characterize them in terms of the given area by first variation techniques. Angles at which minimal boundaries intersect satisfy the standard 120-degree rule up to a suitable change of coordinates. While for $\alpha = 0$ the Grushin perimeter reduces to the Euclidean one and both minimizers coincide with the symmetric double bubble found in [104], for $\alpha = 1$ vertical interface minimizers have Grushin perimeter strictly greater than horizontal interface minimizers. As the latter ones are obtained by translating and dilating the Grushin isoperimetric set found in [131], we conjecture that they solve the double bubble problem with no assumptions on the contact interface.
- In [51] we study the notion of geodesic curvature of smooth horizontal curves parametrized by arc-length in the Heisenberg group, that is the simplest sub-Riemannian structure. Our goal is to give a metric interpretation of this notion of geodesic curvature as the first corrective term in the Taylor expansion of the distance between two close points of the curve.

We would also like to mention the defense of the PhD thesis of Ludovic Saccchelli [3] on the subject.

6.2. Quantum control: new results

Let us list here our new results in quantum control theory.

- In [5] we consider a quantum particle in a potential $V(x)$ ($x \in \mathbb{R}^N$) in a time-dependent electric field $E(t)$ (the control). Boscain, Caponigro, Chambrion and Sigalotti proved in [83] that, under generic assumptions on V, this system is approximately controllable on the $L^2(\mathbb{R}^N, \mathbb{C})$-sphere, in sufficiently large time T. In the present article we show that approximate controllability does not hold in arbitrarily small time, no matter what the initial state is. This generalizes our previous result for Gaussian initial conditions. Moreover, we prove that the minimal time can in fact be arbitrarily large.
- In [11] 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.
- In [14] we consider the one dimensional Schrödinger equation with a bilinear control and prove the rapid stabilization of the linearized equation around the ground state. The feedback law ensuring the rapid stabilization is obtained using a transformation mapping the solution to the linearized equation on the solution to an exponentially stable target linear equation. A suitable condition is imposed on the transformation in order to cancel the non-local terms arising in the kernel system. This conditions also insures the uniqueness of the transformation. The continuity and invertibility of the transformation follows from exact controllability of the linearized system.
- In [33] we discuss how to control a parameter-dependent family of quantum systems. Our technique is based on adiabatic approximation theory and on the presence of curves of conical eigenvalue intersections of the controlled Hamiltonian. As particular cases, we recover chirped pulses for two-level quantum systems and counter-intuitive solutions for three-level stimulated Raman adiabatic passage (STIRAP). The proposed technique works for systems evolving both in finite-dimensional and infinite-dimensional Hilbert spaces. We show that the assumptions guaranteeing ensemble controllability are structurally stable with respect to perturbations of the parametrized family of systems.

6.3. Stability and uncertain dynamics: new results

Let us list here our new results about stability and stabilization of control systems, on the properties of systems with uncertain dynamics.

- In [8] we consider a one-dimensional controlled reaction-diffusion equation, where the control acts on the boundary and is subject to a constant delay. Such a model is a paradigm for more general parabolic systems coupled with a transport equation. We prove that it is possible to stabilize (in H^1 norm) this process by means of an explicit predictor-based feedback control that is designed from a finite-dimensional subsystem. The implementation is very simple and efficient and is based on standard tools of pole-shifting. Our feedback acts on the system as a finite-dimensional predictor. We compare our approach with the backstepping method.
- In [14] we consider the one dimensional Schrödinger equation with a bilinear control and prove the rapid stabilization of the linearized equation around the ground state. The feedback law ensuring the rapid stabilization is obtained using a transformation mapping the solution of the linearized equation to the solution of an exponentially stable target linear equation. A suitable condition is imposed on the transformation in order to cancel the non-local terms arising in the kernel system. This conditions also insures the uniqueness of the transformation. The continuity and invertibility of the transformation follows from exact controllability of the linearized system.
- Based on the notion of generalized homogeneity, we develop in [17] a new algorithm of feedback control design for a plant modeled by a linear evolution equation in a Hilbert space with a possibly unbounded operator. The designed control law steers any solution of the closed-loop system to zero in a finite time. Method of homogeneous extension is presented in order to make the developed control design principles to be applicable for evolution systems with non-homogeneous operators. The design scheme is demonstrated for heat equation with the control input distributed on the segment $[0, 1]$.
- In [19] we analyse the asymptotic behaviour of integro-differential equations modeling N populations in interaction, all structured by different traits. Interactions are modeled by non-local terms involving linear combinations of the total number of individuals in each population. These models have already been shown to be suitable for the modeling of drug resistance in cancer, and they generalise the usual Lotka–Volterra ordinary differential equations. Our aim is to give conditions under which there is persistence of all species. Through the analysis of a Lyapunov function, our first main result gives a simple and general condition on the matrix of interactions, together with a convergence rate. The second main result establishes another type of condition in the specific case of mutualistic interactions. When either of these conditions is met, we describe which traits are asymptotically selected.
- The goal of [20] is to compute a boundary control of reaction-diffusion partial differential equation. The boundary control is subject to a constant delay, whereas the equation may be unstable without any control. For this system equivalent to a parabolic equation coupled with a transport equation, a prediction-based control is explicitly computed. To do that we decompose the infinite-dimensional system into two parts: one finite-dimensional unstable part, and one stable infinite-dimensional part. A finite-dimensional delay controller is computed for the unstable part, and it is shown that this controller succeeds in stabilizing the whole partial differential equation. The proof is based on a an explicit form of the classical Artstein transformation, and an appropriate Lyapunov function. A numerical simulation illustrate the constructive design method.
- [27] focuses on the (local) small-time stabilization of a Korteweg-de Vries equation on bounded interval, thanks to a time-varying Dirichlet feedback law on the left boundary. Recently, backstepping approach has been successfully used to prove the null controllability of the corresponding linearized system, instead of Carleman inequalities. We use the “adding an integrator" technique to gain regularity on boundary control term which clears the difficulty from getting stabilization in small-time.
- Motivated by improved ways to disrupt brain oscillations linked to Parkinson’s disease, we propose

in [29] an adaptive output feedback strategy for the stabilization of nonlinear time-delay systems evolving on a bounded set. To that aim, using the formalism of input-to-output stability (IOS), we first show that, for such systems, internal stability guarantees robustness to exogenous disturbances. We then use this feature to establish a general result on scalar adaptive output feedback of time-delay systems inspired by the "σ-modification" strategy. We finally apply this result to a delayed neuronal population model and assess numerically the performance of the adaptive stimulation.

- In [35] we consider open channels represented by Saint-Venant equations that are monitored and controlled at the downstream boundary and subject to unmeasured flow disturbances at the upstream boundary. We address the issue of feedback stabilization and disturbance rejection under Proportional-Integral (PI) boundary control. For channels with uniform steady states, the analysis has been carried out previously in the literature with spectral methods as well as with Lyapunov functions in Riemann coordinates. In [35], our main contribution is to show how the analysis can be extended to channels with non-uniform steady states with a Lyapunov function in physical coordinates.
- In [37], we study the exponential stabilization of a shock steady state for the inviscid Burgers equation on a bounded interval. Our analysis relies on the construction of an explicit strict control Lyapunov function. We prove that by appropriately choosing the feedback boundary conditions, we can stabilize the state as well as the shock location to the desired steady state in H^2-norm, with an arbitrary decay rate.
- Given a discrete-time linear switched system $\Sigma(A)$ associated with a finite set A of matrices, we consider in [40] the measures of its asymptotic behavior given by, on the one hand, its deterministic joint spectral radius $\rho_d(A)$ and, on the other hand, its probabilistic joint spectral radii $\rho_p(v, P, A)$ for Markov random switching signals with transition matrix P and a corresponding invariant probability v. Note that $\rho_d(A)$ is larger than or equal to $\rho_p(v, P, A)$ for every pair (v, P). In this paper, we investigate the cases of equality of $\rho_d(A)$ with either a single $\rho_p(v, P, A)$ or with the supremum of $\rho_p(v, P, A)$ over (v, P) and we aim at characterizing the sets A for which such equalities may occur.
- In [41], we introduce a method to get necessary and sufficient stability conditions for systems governed by 1-D nonlinear hyperbolic partial-differential equations with closed-loop integral controllers, when the linear frequency analysis cannot be used anymore. We study the stability of a general nonlinear transport equation where the control input and the measured output are both located on the boundaries. The principle of the method is to extract the limiting part of the stability from the solution using a projector on a finite-dimensional space and then use a Lyapunov approach. We improve a result of Trinh, Andrieu and Xu, and give an optimal condition for the design of the controller. The results are illustrated with numerical simulations where the predicted stable and unstable regions can be clearly identified.
- In [44] we construct explicit time-varying feedback laws leading to the global (null) stabilization in small time of the viscous Burgers equation with three scalar controls. Our feedback laws use first the quadratic transport term to achieve the small-time global approximate stabilization and then the linear viscous term to get the small-time local stabilization.
- In [46] we address the question of the exponential stability for the C^1 norm of general 1-D quasilinear systems with source terms under boundary conditions. To reach this aim, we introduce the notion of basic C^1 Lyapunov functions, a generic kind of exponentially decreasing function whose existence ensures the exponential stability of the system for the C^1 norm. We show that the existence of a basic C^1 Lyapunov function is subject to two conditions: an interior condition, intrinsic to the system, and a condition on the boundary controls. We give explicit sufficient interior and boundary conditions such that the system is exponentially stable for the C^1 norm and we show that the interior condition is also necessary to the existence of a basic C^1 Lyapunov function. Finally, we show that the results conducted in this article are also true under the same conditions for the exponential stability in the C^p norm, for any $p \geq 1$.

- In [47] we study the exponential stability for the C^1 norm of general 2×2 1-D quasilinear hyperbolic systems with source terms and boundary controls. When the eigenvalues of the system have the same sign, any nonuniform steady-state can be stabilized using boundary feedbacks that only depend on measurements at the boundaries and we give explicit conditions on the gain of the feedback. In other cases, we exhibit a simple numerical criterion for the existence of basic C^1 Lyapunov function, a natural candidate for a Lyapunov function to ensure exponential stability for the C^1 norm. We show that, under a simple condition on the source term, the existence of a basic C^1 (or C^p , for any $p \geq 1$) Lyapunov function is equivalent to the existence of a basic H^2 (or H^q , for any $q \geq 2$) Lyapunov function, its analogue for the H^2 norm. Finally, we apply these results to the nonlinear Saint-Venant equations. We show in particular that in the subcritical regime, when the slope is larger than the friction, the system can always be stabilized in the C^1 norm using static boundary feedbacks depending only on measurements of at the boundaries, which has a large practical interest in hydraulic and engineering applications.
- In [48] we study the exponential stability in the H^2 norm of the nonlinear Saint-Venant (or shallow water) equations with arbitrary friction and slope using a single Proportional-Integral (PI) control at one end of the channel. Using a local dissipative entropy we find a simple and explicit condition on the gain the PI control to ensure the exponential stability of any steady-states. This condition is independent of the slope, the friction, the length of the river, the inflow disturbance and, more surprisingly, the steady-state considered. When the inflow disturbance is time-dependent and no steady-state exist, we still have the Input-to-State stability of the system, and we show that changing slightly the PI control enables to recover the exponential stability of slowly varying trajectories.
- The exponential stability problem of the nonlinear Saint-Venant equations is addressed in [49]. We consider the general case where an arbitrary friction and space-varying slope are both included in the system, which lead to non-uniform steady-states. An explicit quadratic Lyapunov function as a weighted function of a small perturbation of the steady-states is constructed. Then we show that by a suitable choice of boundary feedback controls, that we give explicitly, the local exponential stability of the nonlinear Saint-Venant equations for the H^2-norm is guaranteed.
- [53] elaborates control strategies to prevent clustering effects in opinion formation models. This is the exact opposite of numerous situations encountered in the literature where, on the contrary, one seeks controls promoting consensus. In order to promote declustering, instead of using the classical variance that does not capture well the phenomenon of dispersion, we introduce an entropy-type functional that is adapted to measuring pairwise distances between agents. We then focus on a Hegselmann-Krause-type system and design declustering sparse controls both in finite-dimensional and kinetic models. We provide general conditions characterizing whether clustering can be avoided as function of the initial data. Such results include the description of black holes (where complete collapse to consensus is not avoidable), safety zones (where the control can keep the system far from clustering), basins of attraction (attractive zones around the clustering set) and collapse prevention (when convergence to the clustering set can be avoided).
- In [54] we consider the problem of controlling parabolic semilinear equations arising in population dynamics, either in finite time or infinite time. These are the monostable and bistable equations on $(0, L)$ for a density of individuals $0 \leq y(t, x) \leq 1$, with Dirichlet controls taking their values in $[0, 1]$. We prove that the system can never be steered to extinction (steady state 0) or invasion (steady state 1) in finite time, but is asymptotically controllable to 1 independently of the size L, and to 0 if the length L of the interval domain is less than some threshold value L^*, which can be computed from transcendental integrals. In the bistable case, controlling to the other homogeneous steady state $0 < \theta < 1$ is much more intricate. We rely on a staircase control strategy to prove that θ can be reached in finite time if and only if $L < L^?$. The phase plane analysis of those equations is instrumental in the whole process. It allows us to read obstacles to controllability, compute the threshold value for domain size as well as design the path of steady states for the control strategy.
- Given a linear control system in a Hilbert space with a bounded control operator, we establish in [56] a characterization of exponential stabilizability in terms of an observability inequality.

Such dual characterizations are well known for exact (null) controllability. Our approach exploits classical Fenchel duality arguments and, in turn, leads to characterizations in terms of observability inequalities of approximately null controllability and of α-null controllability. We comment on the relationships between those various concepts, at the light of the observability inequalities that characterize them.

- In [58] we use the backstepping method to study the stabilization of a 1-D linear transport equation on the interval $(0, L)$, by controlling the scalar amplitude of a piecewise regular function of the space variable in the source term. We prove that if the system is controllable in a periodic Sobolev space of order greater than 1, then the system can be stabilized exponentially in that space and, for any given decay rate, we give an explicit feedback law that achieves that decay rate.

Let us also mention the lecture notes [31] on stabilization of semilinear PDE's, which have been published this year.

6.4. Optimal control: new results

Let us list here our new results in optimal control theory beyond the sub-Riemannian framework.

- In [4] we focus on regional deterministic optimal control problems, i.e., problems where the dynamics and the cost functional may be different in several regions of the state space and present discontinuities at their interface. Under the assumption that optimal trajectories have a locally finite number of switchings (no Zeno phenomenon), we use the duplication technique to show that the value function of the regional optimal control problem is the minimum over all possible structures of trajectories of value functions associated with classical optimal control problems settled over fixed structures, each of them being the restriction to some submanifold of the value function of a classical optimal control problem in higher dimension. The lifting duplication technique is thus seen as a kind of desingularization of the value function of the regional optimal control problem. In turn, we extend to regional optimal control problems the classical sensitivity relations and we prove that the regularity of this value function is the same (i.e., is not more degenerate) than the one of the higher-dimensional classical optimal control problem that lifts the problem.
- The goal of [9] is to show how non-parametric statistics can be used to solve some chance constrained optimization and optimal control problems. 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. We then show how this technique can be applied and implemented for a class of problems including the Goddard problem and the trajectory optimization of an Ariane 5-like launcher.
- In control theory the term chattering is used to refer to fast oscillations of controls, such as an infinite number of switchings over a finite time interval. In [10] we focus on three typical instances of chattering: the Fuller phenomenon, referring to situations where an optimal control features an accumulation of switchings in finite time; the Robbins phenomenon, concerning optimal control problems with state constraints, where the optimal trajectory touches the boundary of the constraint set an infinite number of times over a finite time interval; and the Zeno phenomenon, for hybrid systems, referring to a trajectory that depicts an infinite number of location switchings in finite time. From the practical point of view, when trying to compute an optimal trajectory, for instance, by means of a shooting method, chattering may be a serious obstacle to convergence. In [10] we propose a general regularization procedure, by adding an appropriate penalization of the total variation. This produces a family of quasi-optimal controls whose associated cost converge to the optimal cost of the initial problem as the penalization tends to zero. Under additional assumptions, we also quantify quasi-optimality by determining a speed of convergence of the costs.
- In [12], a new robust and fast method is developed to perform transfers that minimize fuel consumption between two invariant manifolds of periodic orbits in the circular restricted three-body problem. The method starts with an impulse transfer between two invariant manifolds to build an optimal

control problem. This allows to choose an adequate fixed transfer time. Using the Pontryagin maximum principle, the resolution of the problem is formulated as that of finding the zero of a shooting function (indirect method). The algorithm couples different kinds of continuations (on cost, final state, and thrust) to improve robustness and to initialize the solver. The efficiency of the method is illustrated with numerical examples. Finally, the influence of the transfer time is studied numerically thanks to a continuation on this parameter, and it checks that, when transfer duration goes to zero, the control converges to the impulse transfer that it started with. It shows the robustness of the method and establishes a mathematical link between the two problems.

- In [15] we consider the controllability problem for finite-dimensional linear autonomous control systems, under state constraints but without imposing any control constraint. It is well known that, under the classical Kalman condition, in the absence of constraints on the state and the control, one can drive the system from any initial state to any final one in an arbitrarily small time. Furthermore, it is also well known that there is a positive minimal time in the presence of compact control constraints. We prove that, surprisingly, a positive minimal time may be required as well under state constraints, even if one does not impose any restriction on the control. This may even occur when the state constraints are unilateral, like the nonnegativity of some components of the state, for instance. Using the Brunovsky normal forms of controllable systems, we analyze this phenomenon in detail, that we illustrate by several examples. We discuss some extensions to nonlinear control systems and formulate some challenging open problems.
- In [18] we consider a system of two coupled integro-differential equations modeling populations of healthy and cancer cells under therapy. Both populations are structured by a phenotypic variable, representing their level of resistance to the treatment. We analyse the asymptotic behaviour of the model under constant infusion of drugs. By designing an appropriate Lyapunov function, we prove that both densities converge to Dirac masses. We then define an optimal control problem, by considering all possible infusion protocols and minimising the number of cancer cells over a prescribed time frame. We provide a quasi-optimal strategy and prove that it solves this problem for large final times. For this modeling framework, we illustrate our results with numerical simulations, and compare our optimal strategy with periodic treatment schedules.
- In [21] we use conductance based neuron models and the mathematical modeling of Optogenetics to define controlled neuron models and we address the minimal time control of these affine systems for the first spike from equilibrium. We apply tools of geometric optimal control theory to study singular extremals and we implement a direct method to compute optimal controls. When the system is too large to theoretically investigate the existence of singular optimal controls, we observe numerically the optimal bang-bang controls.
- In [23] we first derive a general integral-turnpike property around a set for infinite-dimensional non-autonomous optimal control problems with any possible terminal state constraints, under some appropriate assumptions. Roughly speaking, the integral-turnpike property means that the time average of the distance from any optimal trajectory to the turnpike set converges to zero, as the time horizon tends to infinity. Then, we establish the measure-turnpike property for strictly dissipative optimal control systems, with state and control constraints. The measure-turnpike property, which is slightly stronger than the integral-turnpike property, means that any optimal (state and control) solution remains essentially, along the time frame, close to an optimal solution of an associated static optimal control problem, except along a subset of times that is of small relative Lebesgue measure as the time horizon is large. Next, we prove that strict strong duality, which is a classical notion in optimization, implies strict dissipativity, and measure-turnpike. Finally, we conclude the paper with several comments and open problems.
- In [24], we investigate the asymptotic behavior of optimal designs for the shape optimization of 2D heat equations in long time horizons. The control is the shape of the domain on which heat diffuses. The class of 2D admissible shapes is the one introduced by Sverák, of all open subsets of a given bounded open set, whose complementary sets have a uniformly bounded number of connected components. Using a Γ-convergence approach, we establish that the parabolic optimal

designs converge as the length of the time horizon tends to infinity, in the complementary Hausdorff topology, to an optimal design for the corresponding stationary elliptic equation.

- In [25], we study the steady-state (or periodic) exponential turnpike property of optimal control problems in Hilbert spaces. The turnpike property, which is essentially due to the hyperbolic feature of the Hamiltonian system resulting from the Pontryagin maximum principle, reflects the fact that, in large time, the optimal state, control and adjoint vector remain most of the time close to an optimal steady-state. A similar statement holds true as well when replacing an optimal steady-state by an optimal periodic trajectory. To establish the result, we design an appropriate dichotomy transformation, based on solutions of the algebraic Riccati and Lyapunov equations. We illustrate our results with examples including linear heat and wave equations with periodic tracking terms.
- The Allee threshold of an ecological system distinguishes the sign of population growth either towards extinction or to carrying capacity. In practice human interventions can tune the Allee threshold for instance thanks to the sterile male technique and the mating disruption. In [26] we address various control objectives for a system described by a diffusion-reaction equation regulating the Allee threshold, viewed as a real parameter determining the unstable equilibrium of the bistable nonlinear reaction term. We prove that this system is the mean field limit of an interacting system of particles in which individual behaviours are driven by stochastic laws. Numerical simulations of the stochastic process show that population propagations are governed by wave-like solutions corresponding to traveling solutions of the macroscopic reaction-diffusion system. An optimal control problem for the macroscopic model is then introduced with the objective of steering the system to a target traveling wave. The relevance of this problem is motivated by the fact that traveling wave solutions model the fact that bounded space domains reach asymptotically an equilibrium configuration. Using well known analytical results and stability properties of traveling waves, we show that well-chosen piecewise constant controls allow to reach the target approximately in sufficiently long time. We then develop a direct computational method and show its efficiency for computing such controls in various numerical simulations. Finally we show the efficiency of the obtained macroscopic optimal controls in the microscopic system of interacting particles and we discuss their advantage when addressing situations that are out of reach for the analytical methods. We conclude the article with some open problems and directions for future research.
- Consider a general nonlinear optimal control problem in finite dimension, with constant state and/or control delays. By the Pontryagin Maximum Principle, any optimal trajectory is the projection of a Pontryagin extremal. In [39] we establish that, under appropriate assumptions, Pontryagin extremals depend continuously on the parameter delays, for adequate topologies. The proof of the continuity of the trajectory and of the control is quite easy, however, for the adjoint vector, the proof requires a much finer analysis. The continuity property of the adjoint with respect to the parameter delay opens a new perspective for the numerical implementation of indirect methods, such as the shooting method. We also discuss the sharpness of our assumptions.
- In [43] we are concerned about the controllability of a general linear hyperbolic system of the form $\partial_t w(t,x) = \Sigma(x)\partial_x w(t,x) + \gamma C(x) w(t,x)$ ($\gamma \in \mathbb{R}$) in one space dimension using boundary controls on one side. More precisely, we establish the optimal time for the null and exact controllability of the hyperbolic system for generic γ. We also present examples which yield that the generic requirement is necessary. In the case of constant Σ and of two positive directions, we prove that the null-controllability is attained for any time greater than the optimal time for all $\gamma \in \mathbb{R}$ and for all C which is analytic if the slowest negative direction can be alerted by both positive directions. We also show that the null-controllability is attained at the optimal time by a feedback law when $C \equiv 0$. Our approach is based on the backstepping method paying a special attention on the construction of the kernel and the selection of controls.
- In [52] we consider a state-constrained optimal control problem of a system of two non-local partial-differential equations, which is an extension of the one introduced in a previous work in mathematical oncology. The aim is to minimize the tumor size through chemotherapy while avoiding the emergence of resistance to the drugs. The numerical approach to solve the problem was the

combination of direct methods and continuation on discretization parameters, which happen to be insufficient for the more complicated model, where diffusion is added to account for mutations. In [52], we propose an approach relying on changing the problem so that it can theoretically be solved thanks to a Pontryagin Maximum Principle in infinite dimension. This provides an excellent starting point for a much more reliable and efficient algorithm combining direct methods and continuations. The global idea is new and can be thought of as an alternative to other numerical optimal control techniques.

We would also like to mention the defense of the PhD theses of Riccardo Bonalli [1] and Antoine Olivier [2] on the subject.

COMMANDS Project-Team

7. New Results

7.1. Optimal control of ODEs

7.1.1. Optimal healh insurance design

In [7] we analyze the design of optimal medical insurance under ex post moral hazard, i.e., when illness severity cannot be observed by insurers and policyholders decide for themselves on their health expenditures. The trade-off between ex anterisk sharing and ex post incentive compatibility is analyzed in an optimal revelation mechanism under hidden information and risk aversion. The optimal contract provides partial insurance at the margin, with a deductible when insurers' rates are affected by a positive loading, and it may also include an upper limit on coverage. The potential to audit the health state leads to an upper limit on out-of-pocket expenses.

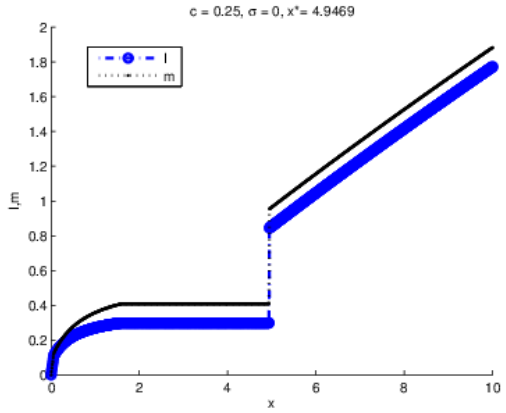


Figure 1.

Health insurance with audit. The 'out-of-pocket' expense ($m - l$) remains bounded.

7.1.2. Optimal Battery Aging: an Adaptive Weights Dynamic Programming Algorithm

In [5] we present an algorithm to handle the optimization over a long horizon of an electric microgrid including a battery energy storage system. While the battery is an important and costly component of the microgrid, its aging process is often not taken into account by the Energy Management System, mostly because of modeling and computing challenges. We address the computing aspect by a new approach combining dynamic programming, decomposition and relaxation techniques. We illustrate this 'adaptive weight' method with numerical simulations for a toy microgrid model. Compared to a straightforward resolution by dynamic programming, our algorithm decreases the computing time by more than one order of magnitude, can be parallelized, and allows for online implementations. We believe that this approach can be used for other applications presenting fast and slow variables.

Optimal battery aging. Comparison of brute-force and adaptive weights algorithm.

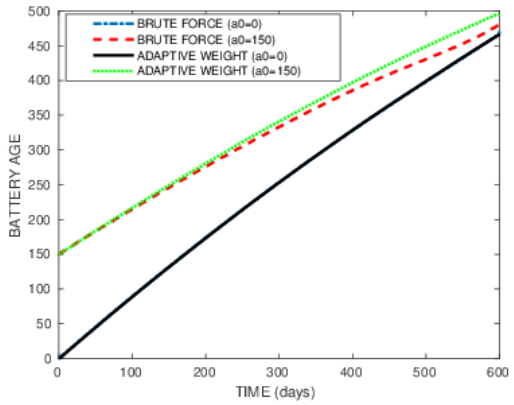


Figure 2.

7.1.3. Aircraft model identification and trajectory optimization

During the PhD of C. Rommel co-supervised with startup Safety Line, we investigated several formulations and methods for identifying an aircraft dynamics from recorded flight data. In particular, in [14] we introduce a block-sparse Bolasso approach for variable selection. In [12] we study how to quantify the closedness of a trajectory to a set of reference ones, based on the meean marginal likelihood. These works are combined with a gaussian mixture model in [15], allowing for a trade-off between optimality and acceptability of the aircraft trajectories.

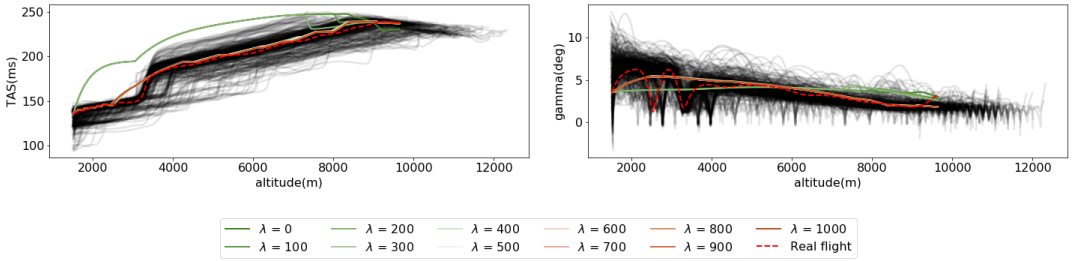


Figure 3.

Aircraft trajectory optimization. Illustration of the trade-off between performance (consumption) and acceptability (weighted by λ).

7.1.4. Microalgae cultivation in a turbid medium

In the context of IPL Algae in Silico, we study in [11] the cultivation of microalgae in a turbid medium. Microalgae cultivation with wastewater is a promising way of reducing the energetic needs for wastewater treatment and the costs of biofuel production. However, the very turbid medium is not favorable for the development of microalgae. Indeed, light, the key element for photosynthesis, rapidly vanishes along depth due

to absorption and scattering. Therefore it is crucial to understand the effects of the depth on turbid cultures. In this work, we study theoretically the long-term behavior of a continuous culture of microalgae exposed to a periodic source of light. By allowing periodic variations of the depth and the hydraulic retention time, we show that the microalgae population is forced to a periodic regime. Finally, we address numerically the problem of determining the optimal variations of the depth and the hydraulic retention time for maximizing the productivity of the culture in the periodic regime.

7.1.5. Optimizing running a race on a curved track

Following on a previous study of optimal running strategies [16], we investigate in [9] the case of a curved track. In order to determine the optimal strategy to run a race on a curved track according to the lane number, we introduce a model based on differential equations for the velocity, the propulsive force and the anaerobic energy which takes into account the centrifugal force. This allows us to analyze numerically the different strategies according to the different types of track since the straight line is not always of the same length. In particular, we find that the tracks with shorter straight lines lead to better performances, while the double bend track with the longest straight line leads to the worst performances and the biggest difference between lanes. Then for a race with two runners, we introduce a psychological attraction to follow someone just ahead and the delay to benefit again from this interaction after being overtaken. We provide numerical simulations in different cases. Results are overall consistent with the IAAF rules for lanes drawing, indicating that middle lanes are the best, followed by the exterior lanes, interior lanes being the worst.

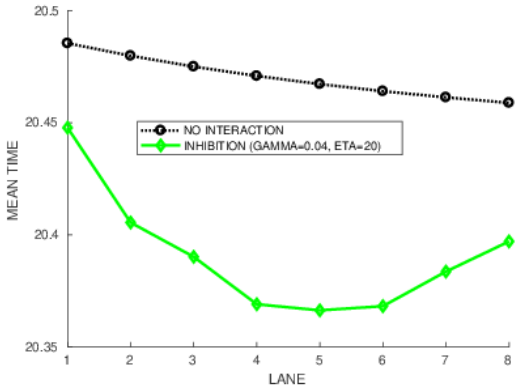


Figure 4.

Running on a curved track. Mean race times per lane, taking into account centrifugal force and psychological interaction.

7.2. Optimal control of PDEs and stochastic control

7.2.1. Sufficient optimality conditions for bilinear optimal control of the linear damped wave equation

In [8] we discuss sufficient optimality conditions for an optimal control problem for the linear damped wave equation with the damping parameter as the control. We address the case that the control enters quadratic in the cost function as well as the singular case that the control enters affine. For the non-singular case we consider strong and weak local minima , in the singular case we derive sufficient optimality conditions for weak local minima. Thereby, we take advantage of the Goh transformation applying techniques recently established in

Aronna, Bonnans, and Kröner [Math. Program. 168(1):717–757, 2018]. Moreover, a numerical example for the singular case is presented.

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

In [3] 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 weigthed Sobolev spaces. This involves a generalization of the commutator analysis introduced by Achdou and Tchou.

7.2.3. Infinite Horizon Stochastic Optimal Control Problems with Running Maximum Cost

In [6] we analyze an infinite horizon stochastic optimal control problem with running maximum cost. The value function is characterized as the viscosity solution of a second-order Hamilton-Jacobi-Bellman (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. These properties are verified for a specific semi-Lagrangian scheme.

7.2.4. A stochastic data-based traffic model applied to vehicles energy consumption estimation

In the framework of the PhD of A. Le Rhun, we present in [10] a new approach to estimate traffic energy consumption via traffic data aggregation in (speed,acceleration) probability distributions. The aggregation is done on each segment composing the road network. In order to reduce data occupancy, clustering techniques are used to obtain meaningful classes of traffic conditions. Different times of the day with similar speed patterns and traffic behavior are thus grouped together in a single cluster. Different energy consumption models based on the aggregated data are proposed to estimate the energy consumption of the vehicles in the road network. For validation purposes, a microscopic traffic simulator is used to generate the data and compare the estimated energy consumption to the reference one. A thorough sensitivity analysis with respect to the parameters of the proposed method (i.e. number of clusters, size of the distributions support, etc.) is also conducted in simulation. Finally, a real-life scenario using floating car data is analyzed to evaluate the applicability and the robustness of the proposed method.

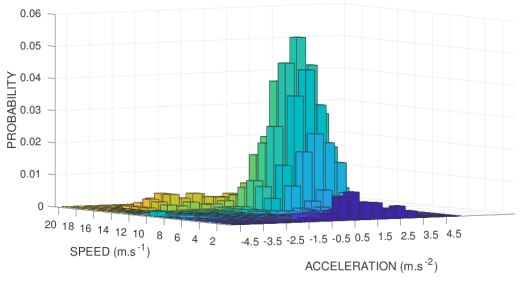


Figure 5.

Traffic modeling. Example of (speed,acceleration) distribution and illustration of clustering results with respect to day time. Slow traffic for yellow and purple clusters clearly corresponds to peak hours.

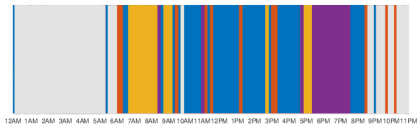

12AM 1AM 2AM 3AM 4AM 5AM 6AM 7AM 8AM 9AM 10AM 11AM 12PM 1PM 2PM 3PM 4PM 5PM 6PM 7PM 8PM 9PM 10PM 11PM

Figure 6.

DISCO Project-Team

6. New Results

6.1. Spectral abscissa characterization for Time-delay systems

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [Université Paris Sud], Thomas Vyhlidal [Czech technical university in Prague], Karim Trabelsi [IPSA].

It is well known that the spectral abscissa of a given dynamical is nothing but the corresponding solutions' exponential decay. The analytical characterization of the spectral abscissa for infinite dimensional dynamical systems is an old problem which is still nowadays a question of ongoing interest due to its links with stability problems. We produced several works in this topic dealing with reduced order retarded Time-delay systems and emphasized a property that we call *multiplicity induced-dominancy*. In the paper [13], the interest of using time-delay in the controller design as a control parameter is underlined and the way to assign a dominant spectral value is demonstrated. As a matter of fact, it is shown that the multiplicity of given spectral value may reach the degree of the corresponding quasipolynomial. Furthermore, when this holds, then using a particular factorization of the quasipolynomial, such a multiple spectral value is shown to be the corresponding spectral abscissa. A generalization of such a result to generic second order retarded equation with a single delay is established in [12]. More precisely, a parametric characterization of the spectral abscissa is established using the principle argument theorem. Furthermore, in the work [45], the potential applicability of such a parametric characterization in controller design in concrete application is demonstrated. As a matter of fact, a third order retarded system modeling the dynamics of Mach number in a wind tunnel is considered and a delayed controller design based on the spectral abscissa assignment is proposed.

6.2. Poles placement for reduced order Time-delay systems

Participants: Souad Amrane [University Mouloud Mammeri], Islam Boussaada, Fazia Bedouhen [University Mouloud Mammeri], Silviu-Iulian Niculescu, Matej Kure [Czech technical university in Prague], Wim Michiels [KU Leuven], Thomas Vyhlidal [Czech technical university in Prague].

It is well known in dynamical system theory that real spectral values correspond to non oscillating solutions. In the paper [11]we made a connexion between the degree of a given quasipolynomial and the admissible number of non oscillating modes for the corresponding Time-delay system. More precisely, we have shown that the assignment of at most n real spectral values is possible for generic quasipolynomial function of degree n. Namely, explicit formulas on the quasipolynomial's coefficients guaranteeing the coexistence of n negative spectral values are obtained. Furthermore, a new quasipolynomial factorization technique, analogous to the one we developed for multiple spectral values for the proof of the dominancy of n distinct negative spectral values is obtained.

In the paper [23] a robust alternative of the delayed resonator is proposed by spectral approach where a double root assignment at the excitation frequency is proposed. Such an excitation frequency is projected to widening the stop-band in the active absorber frequency response. It is shown that the performance sensitivity to the mismatch between the design and true excitation frequency is considerably decreased. Additionally, the overall scheme is supplemented by a control loop which improves the stability margin.

6.3. Asymptotic behavior of critical imaginary roots for retarded differential equations

Participants: Islam Boussaada, Jie Chen [City University of Hong Kong], Liana Felix [Universidad Autonoma de San Luis Potosi], Keqin Gu [Southern Illinois University], Fernando Mendez-Barrios [Universidad Autonoma de San Luis Potosi], Dina Irofti, Silviu-Iulian Niculescu, Alejandro Martinez.

The behavior of characteristic roots of time-delay systems, when the delay is subject to small variations is investigated in [26]. We performed an analysis by means of the Weierstrass polynomial which are employed to study the stability behavior of the characteristic roots with respect to small variations on parameters. Analytic description and splitting properties of the Puiseux series expansions of critical roots are characterized by allowing a full description covering all the cases that can be encountered.

In the paper [21] the migration of double imaginary roots of the systems characteristic equation when two parameters are subjected to small deviations is geometrically investigated. Under the least degeneracy assumptions, the local stability crossing curve is shown to have a cusp at the point that corresponds to the double root, which divides the neighborhood of this point into two sectors (called S-sector and a G-sector). We have shown that when the parameters move into the G-sector, one of the roots moves to the right half-plane, and the other moves to the left half-plane. However, when the parameters move into the S-sector, both roots move either to the left half-plane or the right half-plane depending on the sign of a quantity that depends on the characteristic function and its derivatives up to the third order.

6.4. Stability analysis of retarded differential equations with delay-dependent coefficients

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

Retarded dynamical systems with delay dependent coefficients is a class of systems which is frequently encountered in various scientific and engineering applications. The paper [36] provides an overview of the stability analysis of such systems which generalizes those on systems with delay-independent coefficients. Methods of analysis for systems with a single delay and commensurate delays are presented, their application to output feedback control and a geometric perspective that establishes a link between systems with and without delay-dependent coefficients.

The paper [22] presents a systematic method to analyse the stability of systems with single delay in which the coefficient polynomials of the characteristic equation depend on the delay. With respect to the literature on the topic, a less restrictive method to analyse stability is presented. It is found that a much richer behavior is possible when the restrictive assumptions are removed. The interval of interest for the delay is partitioned into subintervals so that the magnitude condition generates a fixed number of frequencies as functions of the delay within each subinterval. The crossing conditions are expressed in a general form, and a simplified derivation for the first-order derivative criterion is obtained.

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

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

Through an LMI approach it was possible to determine envelopes and use them not only to study stability but to design robust controllers for retarded and neutral time-delay systems. The controller designed is robust to parametric uncertainties and can guarantee delay independant stability or delay-dependant $\alpha - stability$ [46].

6.6. Some remarks on the Walton and Marshall method for neutral delay systems

Participants: Catherine Bonnet, Islam Boussaada, Le Ha Vy Nguyen, Marianne Souaiby.

The Walton and Marshall method allows to determine stability windows of delay systems of the retarded and neutral type. We noticed that some delay systems of the neutral type do not behave as claimed in [66] and analyzed carefully the position of the poles of such systems in the right half-plane.

6.7. Local Analysis of Lurie Systems

Participants: Elena Panteley [L2S,CNRS], Stephen Duncan [University of Oxford], Thomas Lathuiliere [University of Oxford], Giorgio Valmorbida.

An important aspect of nonlinear systems is the fact that stability might only be a local property. This means that associated to a stable equilibrium point or periodic trajectory, there is a region of attraction. Such a region is formed by points of trajectories converging to the stable sets. An important task of practical interest is then to estimate these regions via numerical methods that rely on the model of the system. As an illustration, it might be of interest to know the region of safe operation of an electric motor in order to preserve its integrity or, in the case of an autonomous vehicle, limit the operating condition for safety purposes.

For the particular class of Lurie systems, namely systems defined by the interconnection of a linear system and a static nonlinearity, it is possible to compute estimates based on sector inequalities characterizing the nonlinearities in the system. If further information, such as the slope of the nonlinearity is available, one can better characterize local properties such as regions of stability, and input-output relations such as reachable sets and local nonlinear gains.

To obtain these characterizations we rely on numerical methods based on convex optimization. These methods are based on the solution of Lyapunov inequalities yielding Lyapunov functions that are quadratic on both the states and the nonlinearity and has an integral term on the nonlinearity [39].

Moreover, whenever a more precise characterization of the nonlinearity is at hand as for instance nonlinearities having rational Jacobian, one can generalize the local analysis methods using polynomial optimization. This includes the case of standard Lurie systems by considering the interconnection of a polynomial system with static sector nonlinearities that have rational Jacobian. In this setting we have proposed conditions that relax the requirement on the candidate Lyapunov function [17], which serve as stability certificates, from being sum-of-squares of polynomial with respect to the nonlinearities and the Lurie-Postnikov terms from being non-negative.

Further to the stability analysis we were interested in another important phenomenon and its analysis through numerical methods : the existence of limit cycles on nonlinear systems. Such a phenomenon is relevant since it can be used as a method to design stable oscillators with known amplitude and frequency but also to evaluate and suppress undesirable oscillations in engineered systems. In order to proceed with this analysis we have limited our attention to a particular class of systems defined by a Liénard systems and formulate sufficient conditions for existence and uniqueness of limit cycles for systems with a non-differentiable vector field. As an application we consider the example of a linear system with saturation [24]. Moreover, for planar saturating systems we present sufficient conditions for the existence of periodic orbits and we characterize inner and outer sets bounding the periodic orbits. A method to build these bounds, based on the solution to a convex optimization problem is proposed and numerical examples optimizing the region bounding the limit cycle illustrate the technique [25].

6.8. New advances on backstepping

Participants: Frederic Mazenc, Michael Malisoff [LSU], Laurent Burlion [ONERA Toulouse], Jerome Weston [LSU].

We worked on the problem of improving a fundamental control design technique for nonlinear systems called backstepping by using a fundamentally new approach which consists in introducing in the control artificial delays or using dynamic extensions.

In [28], we provided backstepping results for a large class of partially linear systems with an arbitrarily large number of integrators. We proposed control laws whose size respects some constaints given a priori. The key tool is a dynamic extension that contains only one artificial delay, which is in sharp contrast with our prior contributions. We also showed that the closed-loop system is robust, in the input-to-state stability sense, with respect to a large class of model uncertainties, and robust with respect to delays in the measurements. We illustrated the result using an example that is beyond the scope of classical backstepping.

The paper [57] also provides a crucial backstepping result. We explained how globally asymptotically stabilizing output feedbacks can be constructed for a family of nonlinear systems using only a dynamic extension and a "Converging Input-Converging State" assumption and no additional delays. The technique presents several advantages. It provides control laws whose expressions are simple. It makes it possible to stabilize systems in the presence of uncertain terms, which are not necessarily of class C^1 and which prevent the use of the classical backstepping technique. It applies in cases where only part of the state variables can be measured.

6.9. Time-varying systems with delay and Switched Systems

Participants: Frederic Mazenc, Michael Malisoff [LSU], Saeed Ahmed [Inria], Hitay Ozbay [Blikent University, Turkey].

The family of the switched systems is frequently encountered in practice. It can be used to approximate time-varying systems to ease their stability analysis or control.

In [29] we provided theoretical results for the stability and robustness analysis of nonlinear switched time-varying systems with uncertainties and time-varying delays. The delays are allowed to be discontinuous and arbitrarily long with known upper bounds. We established the results via an adaptation of Halanay's inequality and a trajectory based technique. Also, we used the results for designing switched controllers that stabilize linear time-varying systems with time-varying delays.

The contribution [10] proposed a new technique of construction of observers making possible to stabilize by output feedback a class of continuous-time switched linear systems with a time-varying delay in the output. The motivation of this paper is strong: frequently measurements are affected by pointwise time-varying delays. For stability analysis, we developped an extension of the trajectory based approach. A stability condition is given in terms of the upper bound on the time-varying delay to ensure global exponential stability of the switched feedback systems. It is worth observing that the main result applies in cases where some of the subsystems of the switched system are not stabilizable and not detectable.

The paper [27] is also devoted to classes of nonlinear time-varying continuous-time systems with outputs. For a first family of systems, we builded an observer in the case where a state dependent disturbance affects the linear approximation. A fundamental feature of our observer is the fact that it converges after a predetermined finite time. When the disturbances are the zero functions, it provides exact values of the state and it provides an approximate estimate when there are nonzero disturbances. We used this construction to design a globally exponentially stabilizing dynamic output feedback for a second family of nonlinear systems whose outputs are only available on some finite time intervals. Our technique consists in switching between control laws. We applied the control design to the controlled Mathieu equation, which arises in the study of vibrations of an elliptic membrane.

The paper [38] is devoted to a stability analysis for a class of nonlinear systems with a time-varying delay taking both large and small values in an alternating manner, precluding the application of most of the classical control design techniques. The type of assumption we imposed is the following: we imposed on the delay to be "small" on "long" time intervals and possibly "large" on "small" time-intervals. Bearing in mind this key property, we first introduced the concept of delay-hybrid-dependent stability, which grasps the features of the delays described above and represented the studied system as a system with a switched delay. Then by using switching techniques and Lyapunov-Krasovskii functionals (LKFs), we provided a new stability criterion.

6.10. Observers

Participants: Frederic Mazenc, Michael Malisoff [LSU], Saeed Ahmed [Inria], Ali Zemouche [CRAN], Rajesh Rajamani [University of Minneapolis, USA], Maruthi Akella [University of Texas, USA].

We produced several works which pertain to the case where only a part of the state variables can be measured.

In the paper [58], we adopted a technique based on the indroduction of several observers in cascade (such a cascade is called 'sequential observer') for a class of time-varying linear systems in which the inputs and outputs containing sampling and arbitrarily long delays. The observers are of a continuous-discrete type. We used the observers to design controllers that ensure a strong robustness property with respect to uncertainties in the system and the output, under delays and sampling. A fundamental aspect of the approach is that it produces the observers and controllers without distributed terms. We have assessed the performance of the control laws through two examples, which inlcude a DC motor model that illustrates the utility of the work in engineering applications.

In two papers, we developped the theory of the finite time observers. In [53], we study a class of linear continuous-time time-varying systems with piecewise continuous disturbances and piecewise constant outputs. Under a classical assumption of observability, we designed a new type of observers to estimate the solutions of the system in a predetermined finite time. In contrast to the well-established finite time observer design techniques which estimate the system state using a continuous output, our proposed observer applies when only piecewise constant measurements are available. In [54], we construct finite-time reduced order observers for a broad family of nonlinear time-varying continuous-time systems. The motivation for this is the fact that in practice the time-varying aspect of a system may be an obstacle to the design of full-order finite-time observers, but not for the design of reduced order ones. We illustrated our results using a tracking problem for nonholonomic systems in chained form.

Two of our works present construction of asymptotic observers without delay. The paper [61] solves an H_∞ observer design problem for a class of descriptor nonlinear systems. The method we established is theoretical and can be applied to many automatic control design problems such as unknown input estimation problem, which plays an important role in control systems, namely for diagnosis and fault tolerant control. The design relies on the Linear Matrix Inequality condition (LMI) technique. We applied our resut to a model of a flexible joint robot system.

The work [16] is dedicated to the design of a smooth six-degree-of-freedom observer to estimate the incorporating linear and angular velocity, called dual angular velocity, for a rigid body. The approach is based on the dual-quaternion description and we proved that the estimation errors exhibit asymptotic convergence. Furthermore, to achieve tracking control objective, we combined the proposed observer with an independently designed proportional-derivative-like feedback control law (using full-state feedback), and a special Lyapunov "strictification" process is employed to ensure a separation property between the observer and the controller. We performed numerical simulations for a prototypical spacecraft hovering mission application.

6.11. Stabilization of various systems with pointwise delays

Participants: Frederic Mazenc, Michael Malisoff [LSU], Delphine Bresch-Pietri [Mines Paris Tech.], Nicolas Petit [Mines Paris Tech.], Robledo Gonzalo [Univ. de Chile, Chile], Maruthi Akella [University of Texas, USA], Xi-Ming Sun [Dalian University of Technology, China], Xue-Fan Wang [Dalian University of Technology, China].

The presence of delays to big for being neglected is an obstacle to the design of stabilizing controllers in many cases. We have made efforts to overcome this challenge by developping several techniques.

In the paper [14], we investigated the design of a prediction-based controller for a linear system subject to a problematic time-varying input delay: the delay we considered is not necessarily "First-In/First-Out". The feedback law we proposed uses the current delay value in the prediction. It does not exactly compensate the delay in the closed-loop dynamics but does not require to predict future delay values, contrary to classical prediction techniques. Modeling the input delay as a transport Partial Differential Equation, we proved asymptotic stabilization of the system state, provided that the average L_2-norm of the first derivative of the delay over some time-window is sufficiently small and that the average time between two discontinuities (average dwell time) is sufficiently large.

In the paper [51], we adopted another type of strategy: we used a new sequential predictors approach to build uniformly globally exponentially stabilizing feedback controls for a large class of linear time-varying systems that contain an arbitrary number of different delays. This allows different delays in different components of the input. We illustrated our work in an example from identification theory, and in an Euler-Lagrange system arising from two-link manipulator systems.

The paper [31] continues our works on the 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. In the presence of delays and uncertainties, we provided bounds on the delays and on the uncertainties that ensure, with respect to uncertainties, the robustness property called "input-to-state stability".

6.12. Low complexity constrained control using higher degree Lyapunov functions

Participants: Sarmad Munir [NTNU, Trondheim], Sorin Olaru, Morten Hovd [NTNU, Trondheim].

Explicit Model Predictive Control often has a complex solution in terms of the number of regions required to define the solution and the corresponding memory requirement to represent the solution in the online implementation. An alternative approach to constrained control is based on the use of controlled contractive sets. However, polytopic controlled contractive sets may themselves be relatively complex, leading to a complex explicit solution, and the polytopic structure can limit the size of the controlled contractive set. Our recent results [33] develop a method to obtain a larger controlled contractive set by allowing higher order functions in the definition of the contractive set, and explores the use of such higer-order contractive sets in controller design leading to a low complexity explicit control formulation.

6.13. Characterization of ultimate bounds for systems with state-dependent disturbances

Participants: Sorin Olaru, Hiroshi Ito [Kyushu Institute of Technology, Japan].

The work [37] pursues a framework of set characterization of dynamical systems with state-dependent disturbances. It aims to propose a new approach to analysis and design of nonlinear systems involving non-differentiability and asymmetric components which hamper application and effectiveness of local linearization methods. Several characterizations of ultimate bounds are developed. The utility of shifting the fix point is formulated as a parametrization of the ultimate bounds.

6.14. Combinatorial Approach towards Multi-Parametric Quadratic Programming based on Characterizing Adjacent Critical Regions

Participants: Parisa Ahmadi-Moshkenani [NTNU, Trondheim], Sorin Olaru, Tor Johansen [NTNU, Trondheim].

Several optimization-based control design techniques can be cast in the form of parametric optimization problems. The multi-parametric quadratic programming (mpQP) represents a popular class often related to the control of constrained linear systems. The complete solution to mpQP takes the form of explicit feedback functions with a piecewise affine structure, valid in polyhedral partitions of the feasible parameter space known as critical regions. The recently proposed combinatorial approach for solving mpQP has shown better efficiency than geometric approaches in finding the complete solution to problems with high dimensions of the parameter vectors. The drawback of this method, on the other hand, is that it tends to become very slow as the number of constraints increases in the problem. This work [9] presents an alternative method for enumerating all optimal active sets in a mpQP based on theoretical properties of adjacent critical regions and their corresponding optimal active sets. Consequently, it results in excluding a noticeable number of feasible

but not optimal candidate active sets from investigation. Therefore, the number of linear programs that should be solved decreases noticeably and the algorithm becomes faster. Simulation results confirm the reliability of the suggested method in finding the complete solution to the mpQPs while decreasing the computational time compared favourably with the best alternative approaches.

6.15. Active vibration damping in a mechanical structures

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [Université Paris Sud], Thomas Vyhlidal [Czech technical university in Prague], Daniela Danciu [University of Craiova].

In the work [13], an aluminium-based flexible structure embedded in a mobile support subjected to an acceleration is considered. Such a flexible beam is equipped with two piezoelectric patches. One of them is used as an actuator and the second acts as a sensor. These patches are supposed to be rigidly bounded on the beam, one on each side, located at the clamped edge. The whole device is called a piezo-actuated beam which is generally modeled by Euler-Bernoulli equations. Finite element modeling is then applied to reduce the PDE system to a linear finite-dimensional system. Then, the peak of resonance of the first bending mode is damped by using a delayed output-feedback controller, without affecting the neglected vibrating modes in the reduced order model. The proposed controller design is based on the spectral abscissa characterization using the multiplicity property.

6.16. Landing of a civil aircraft

Participants: Frederic Mazenc, Michael Malisoff [LSU], Laurent Burlion [ONERA Toulouse], Victor Gibert [Airbus Toulouse].

In this work and the following, we applied the technique of [28] to problems arising from applications. The paper [56] is devoted to the problem of stabilizing a nonlinear system approximated in a neighborhood of the origin by a saturated chain of integrators when the variables are not accurately measured. We used our control design to solve a control problem that arises in the context of vision based landing of a civil aircraft. In [55], we solved the problem of stabilizing a nonlinear system when the variables are not accurately measured and cannot be differentiated. The proposed method was first motivated and thus finally applied to the vision based control problem of a landing airliner.

6.17. Power electronics devices

Participants: Frederic Mazenc, Alessio Iovine [Efficacity, France].

The contribution [50] is distinct from the papers mentioned above because it uses more traditional backstepping tools. It is devoted to power electronics devices. We proposed a nonlinear control law for a DC/DC boost converter dedicated to extract the maximum power from a photovoltaic (PV) array, taking into account the constraints of the control action. We performed simulations on SimPowerSystems to validate how the developed control strategy is able to properly control the converter.

6.18. Wind Farm Distributed PSO-based Control for Constrained Power Generation Maximization

Participants: Nicolo Gionfra [L2S], Guillaume Sandou, Houria Siguerdidjane [L2S], Damien Faille [EDF], Philippe Loevenbruck [EDF].

A novel distributed approach to treat the wind farm (WF) power maximization problem accounting for the wake interaction among the wind turbines (WTs) is presented. Power constraints are also considered within the optimization problem. These are either the WTs nominal power or a maximum allowed power injection, typically imposed by the grid operator. The approach is model-based. Coupled with a distributed architecture it allows fast convergence to a solution, which makes it exploitable for real-time operations. The WF optimization problem is solved in a cooperative way among the WTs by introducing a new distributed particle swarm optimization algorithm, based on cooperative co-evolution techniques. The algorithm is first analyzed for the unconstrained case, where we show how the WF problem can be distributed by exploiting the knowledge of the aerodynamic couplings among the WTs. The algorithm is extended to the constrained case employing Deb's rule. Simulations are carried out on different WFs and wind conditions, showing good power gains and fast convergence of the algorithm. To appear in Rnewable Energy, 2019.

6.19. Wind Farm Distributed PSO-based Control for Constrained Power Generation Maximization

Participants: Sophie Frasnedo [Safran Electronics and Defense], Guillaume Sandou, Gilles Duc [L2S], Philippe Feyel [Safran Electronics and Defense], Cedric Chapuis [Safran Electronics and Defense].

The inertial stabilisation of the line of sight of an imager fixed on a mobile carrier is considered in order to acquire good quality images despite the disturbances generated by the carrier.

A double stage mechanical stabilisation architecture is proposed, where a second stabilisation stage, based on a piezoelectric actuator, is added to the usual structure. The piezoelectric actuator transfer function and hysteresis are characterized through experiments.

In order to design the controllers of both stages, a high-level image quality criterion (the Modulation Transfer Function MTF) is considered, together with design constraints on the main variables of interest. The criterion and the constraints are evaluated by realistic simulations based on some input and noise profiles measured on a real-life system. The MTF evaluation being time-consuming, a Bayesian optimisation method specially dedicated to expensive-to-evaluate functions is used to obtain the parameters of the controllers. The obtain experimental results are displayed and their performances discussed. To appear in the International Journal of Systems and Sciences in 2019.

6.20. Model Identification for Demand-Side Management of District Heating Substations

Participants: Nadine Aoun [L2S, CEA-LITEN, ADEME], Roland Baviere [CEA-LITEN], Mathieu Vallee [CEA-LITEN], Guillaume Sandou.

Demand-Side Management (DSM) strategies, such as load shifting and nighttime set-back, exploit the thermal inertia of buildings to make the operation of District Heating Systems (DHSs) more efficient. The control strategy requires a building model to assess the flexibility of buildings in handling demand modulation, without jeopardizing the thermal comfort. Reduced Order Models (ROMs) with few parameters are often used for this end; in many previous works their parameters have been identified using time-series data including indoor temperature measurements. However, at a city scale and due to privacy rights, such internal signals are usually unavailable. Thereby, identifying the ROM shall rely solely on measurements available at the substation level.

In our work, we develop and demonstrate a method respecting this practical constraint to identify a first and a second order building model. In literature, a rather simplified approach had been proposed to derive a first order building model from substation measurements. We compare the performance of our methodology with respect to the latter, using the same model structure. As for the second order model, its structure is more relevant to account for different dynamics in buildings equipped with hydronic heating systems or featuring important internal thermal inertia. Data used for the identification is restricted to the heat flux delivered from the DHS, both supply and return water temperatures, mass flowrate across the substation's heat-exchangers and the outdoor temperature. Validation of the proposed approach is carried out using a representative white-box model of a building and its substation written in the Modelica language. Implementation of advanced control strategies for DHSs based on this model identification is in prospect.

6.21. Mathematical Modelling of Acute Myeloid Leukemia

Participants: Catherine Bonnet, Jean Clairambault [MAMBA project-team], François Delhommeau [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Walid Djema, Emilia Fridman [Tel-Aviv University], Pierre Hirsch [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Frédéric Mazenc, Hitay Özbay [Bilkent University].

Our 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.

Cells have amazing features that allow them to guide their development paths and determine their individual and collective fates. Dedifferentiation and transdifferentiation (cell plasticity) are little understood phenomena that allow cells to regress from an advanced differentiated state to a less differentiated one, including the case where cells lose their specific function and become stem cells.

We have introduced cell plasticity into a class of mathematical models we are interested in. We explored a new model involving a dedifferentiation function in the case of two cell maturity stages (stem cells and progeny). We have highlighted the role that dedifferentiation may have in the survival of cancer cells during therapy. The latter hypothesis appears to be in line with some medical observations [48].

We have also developed and analyzed a model taking into the account the fact that few cells of the proliferating compartment may be arrested during an unlimited time [49].

6.22. 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.

Migratory fluxes of humains and of insects of various species have favoured the spreading of diseases worldwide. In particular the Ae Aegypti and Ae Albopictus mosquitoes of the Aedes family are vectors able to transmit and spead among humans a variety of diseases: Dengue, Zika, Chikungunya, Yellow fever and the newly discovered Mayaro.

We have continued to analyze SIR models with time-varying parameters to predict dengue epidemics and compared numerical simulations with real data from Dengue epidemics in Rio de Janeiro in order to estimate the infectivity rate and predict what are the periods more at risk of infection [63], [41].

FACTAS Team

6. New Results

6.1. Inverse problems for Poisson-Laplace equations

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

6.1.1. Inverse magnetization issues from planar data

This work has been 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 was 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 geometry 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 2-D case and have no 3-D counterpart as yet.

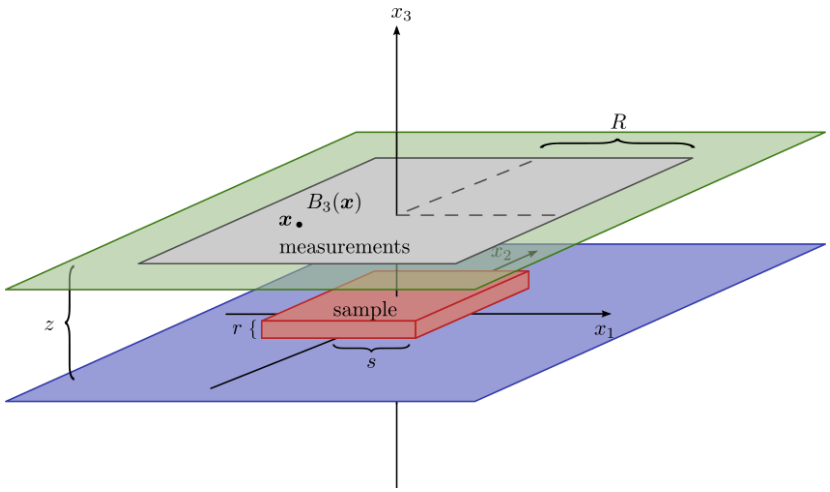


Figure 3. Schematic view of the experimental setup

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 in points of a horizontal square at height z.

We pursued 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 if one measures the field at a distance from the sample.

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 [20], [72]. This year, on the one hand, we conducted with our colleagues at MIT a campaign of fairly systematic tests (with various sensitivity parameters for the sensor, step size between measurement points, overall size of the measurement rectangle, etc.) to observe how our method behaves on true data. The results are overall very good when the signal-to-noise ratio is not poor; however, this revealed a few situations where the observed asymptotics does not fit the theoretical one, and we have currently no clue of the reason of this phenomenon (is it a manipulation error on some of the samples of our campaign? a bug in our implementation? a noise on the data with a surprisingly large effect on the asymptotic? the fact that the asymptotic regime was not yet reached?) Understanding this phenomenon is still an on-going work. On the other hand, we spotted in the literature approaches that are somehow similar to ours: they compute the same integral, but on the whole plane, and try to account for the finiteness of the measurement rectangle by more or less heuristic methods. As the finiteness of the rectangle is built-in in our approach (we exploit the fact the nature of the asymptotic behavior with respect to R is analytically known), we have good hope that our method should compare favorably against its competitors, but we did not conduct systematic tests yet.

The second approach attempts to generalize the previous expansions in the case when R is moderately large (but only in the thin slab framework, modeling the sample as a rectangle). For this purpose, we setup a bounded extremal problem (BEP, see Section 3.3.1) and submitted an article last year on the subject. It has been accepted for publication this year, see [12].

A third approach developed during the previous years was to design an alternate procedure to compute a good linear estimator, dwelling on expansions on a family of piecewise affine functions, with a restricted number of pieces. A key point here is that it is possible to derive explicit formulas for the adjoint operator B_3^* (in appropriate L^2 spaces) to the operator B_3 mapping a magnetization to the vertical component of the field, when applied to polynomials. We derived this year explicit recurrence formulas that allow one to efficiently compute B_3^* of a polynomial of any degree in linear time with respect to the number of monomials. We currently only have draft notes of this research.

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 sharpens in 2-D setting the structure theorem of [76]. Moreover, a characterization of equivalent sources having minimal total variation has been obtained when the support of the magnetization is very scattered (namely: purely 1-unrectifiable, which holds in particular for dipolar models) and also for certain magnetizations of physical 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 the operators relating the magnetization to the field, which prevents them from assuming constant level on large sets. Moreover, we proved that the argument of the minimum of the regularized criterion $\|f-B_3\mu\|_2^2+\lambda\|\mu\|_{TV}$ is unique; here, μ is the measure representing the magnetization with respect to which the criterion gets optimized, f is the data and $\lambda>0$ a regularization parameter, while $\|\mu\|_{TV}$ is the total variation of μ. An implementation is currently being set up with promising results, discretization beforehand on a fixed grid. 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. [21].

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). 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 functions in the Hilbert Hardy space of the upper half-plane. This is the subject of ongoing work with E. Pozzi (Department of Mathematics and Statistics, St Louis Univ., St Louis, Missouri, USA).

For magnetizations supported in a volume Ω 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 Ω there is a unique magnetization supported on $\partial\Omega$ (the balayage of m) and producing the same field outside Ω. Thus, describing silent sources supported on $\partial\Omega$ is a way to factor out some of the complexity of the situation. When m is located in the plane, the Hardy-Hodge decomposition introduced in [35] (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 (resp. above) in their decomposition. When m is supported on a closed compact surface, a similar decomposition exists for $\mathbb{R}^3$-valued vector fields on $\partial\Omega$, (see Section 6.4), that allows us 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 significance and the algorithmic implications of that equation are under study.

Other types of inverse magnetization problems can be tackled using such techniques, in particular global Geomagnetic issues which arise in spherical geometry. In collaboration with C. Gerhards from the Technische Universität Bergakademie Freiberg (Germany), 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 [33]. This assumption is not unrealistic: parts of Australia and of northern Europe are considered as fairly well understood from the magnetostatic view point. We are currently working to test the algorithm against real data, in collaboration with Geophysicists.

6.1.2. Inverse magnetization issues from sparse cylindrical data

The team Factas 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 8.2.1). 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 Factas is to enhance the numerical efficiency of post-processing data obtained with this magnetometer.

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 6.1.3), we try to recover the position and the moment of the dipole using the available measurements. This is still on-going work which constitutes the main topic of the PhD thesis of K. Mavreas.

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 ρ and its azimuth ϕ. We use a rational approximation technique which, for the circle of measurements at height h, gives us an estimate of the complex number $u_h = \frac{1+\rho^2+(h-z)^2}{\rho}\, e^{i\phi}$, from which ϕ is directly obtained. Besides, from the relation $\rho|u_h| = 1+\rho^2+(h-z)^2$, we see that the point (ρ, z) lies on a circle C_h. Therefore, with measurements

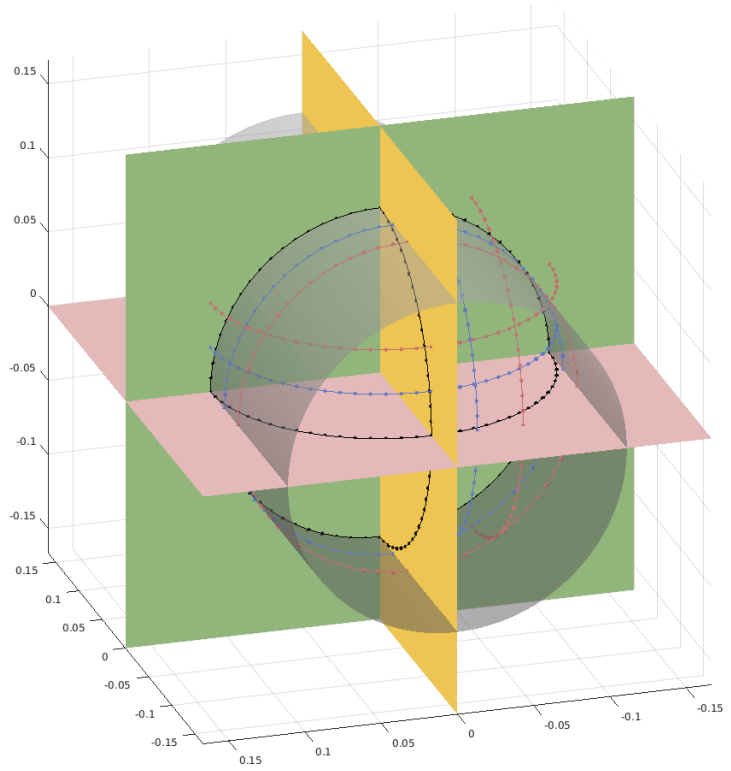


Figure 4. Typical measurements obtained with the instrument of Cerege. Measurements of the field are performed on nine circles, given as sections of three cylinders. On each circle, only one component of the field is measured: the component B_h along the axis of the corresponding cylinder (blue points),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

at three different heights h_i $(i = 1, 2, 3)$, we can in principle recover (ρ, z) as the intersection of the three circles C_{h_1}, C_{h_2} and C_{h_3}.

In practice, due to the many sources of imprecision (the first of all being that the field is not truly generated by a single dipole), the circles do not all truly intersect. This year, we studied three different strategies to estimate the pseudo-intersection point of the circles. In the plane, for a point P and a circle C of center O and radius R, we define $d(P, C) = |\|PO\| - R|$ where $\|\cdot\|$ denotes the Euclidean distance, and $h(P, C) = \|PO\|^2 - R^2$ and we formulate the problem of finding a pseudo-intersection point between C_{h_1}, C_{h_2} and C_{h_3} as either:

1. finding a point P that minimizes $d(P, C_{h_1}) + d(P, C_{h_2}) + d(P, C_{h_3})$;
2. finding a point P for which $h(P, C_{h_1}) = h(P, C_{h_2}) = h(P, C_{h_3})$;
3. finding a point P that minimizes $h(P, C_{h_1})^2 + h(P, C_{h_2})^2 + h(P, C_{h_3})^2$.

The first case turns out to actually be a generalization of two classical concepts: the Fermat point (or Torricelli point) of a triangle, and the Alhazen optical problem. The second case corresponds to a classical notion called the *radical center* of three circles (intersection of the three corresponding radical axes). Finally, the third case does not seem to have a documented solution. We solve it by writing the algebraic system of two equations corresponding to the critical points of the function, after an appropriate change of coordinates in order to reduce the degree. Finally, we get a superset of the solutions by estimating the roots of the resultant of both polynomials. First experiments showed that the third formulation led to the most satisfying estimate of the pseudo-intersection. We also implemented a heuristic numerical procedure (without theoretical formulas for its solution) to estimate the point P that minimizes $d(P, C_{h_1})^2 + d(P, C_{h_2})^2 + d(P, C_{h_3})^2$, and it also gives fairly acceptable estimates. This work has not yet been submitted for publication.

Another important part of our work this year has been to extensively test our implementation of the rational approximation procedure which is at the heart of our method (and which is also used for the problem described in Section 6.1.3). These tests allowed us to detect situations in which the algorithm was falling into an infinite loop or was converging towards a local minimum that was not really the best approximation. It also revealed that all initialization strategies for the iterative optimization algorithm were not equally sensitive to the noise. This led us to redesign our implementation.

Finally, the article that we submitted last year, with a rudimentary approach to recover ρ and z from the data obtained at several heights, has been accepted and will be published soon, see [14].

6.1.3. Inverse problems in medical imaging

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 [7], [40] 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 Matlab version of FS3D, a new (C++) version of the software that automatically performs the estimation of the quantity of sources is being built, specifically this year in the framework of the AMDT Bolis2 (“Action Mutualisée de Développement Technologique”, “Boîte à Outils Logiciels pour l’Identification de Sources”), together with engineers from the SED (Service d’Expérimentation et de Développement) of the Research Center. This new version, still under development, is modular, portable and possesses a nice GUI (using Qt5, dtk, vtk), while non regression (continuous integration) is ensured.

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 from dipolar current sources: for EEG data that correspond to measurements of the electrical potential, one should consider *triple* poles; this will also be the case for MEG – magneto-encephalography – data. However, for (magnetic) field data produced by magnetic dipolar sources, like in Section 6.1.2 , one should consider poles of order five.

Though numerically observed in [8], 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 and will be the topic of further study. 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 INS in Marseille; 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 field (its normal component on the MEG helmet, that can be assumed to be spherical). 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.

Concerning dipolar source estimation from EEG, joint work with Marion Darbas (Univ. Picardie Jules Verne, Laboratoire Amiénois de Mathématique Fondamentale et Appliquée, LAMFA) is in progress for neonates data and models. Their specificity is that the skull does not have a constant conductivity (at the fontanels location, the bone is spongy). We pursue together a study of the influence of the skull conductivity on the inverse EEG problem, using in particular FS3D, see also [70].

We also consider non quasi-static models in order to more precisely analyze the time influence on the behavior of the solutions to the inverse source problems in EEG and MEG. This is current work with Iannis Stratis and Atanasios Yannacopoulos (National and Kapodistrian University of Athens, Greece, Department of Mathematics).

6.2. Matching problems and their applications

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

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. For example, 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. Antennas are not the only systems where matching is of importance: in multiplexer design, one of the most complicated problems among microwave device synthesis, each filter is plugged at one of its accesses on a load made of the common manifold and all other channel filters. This load is far from being matched, and leads to a complex simultaneous matching problem, of all filters connected via the common manifold junction. Our goal is therefore to develop a method for filter synthesis that allows us to match varying loads on specific frequency bands, while enforcing some rejection properties away from the pass-band.

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

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

The matching problem of minimizing $|G_{1,1}|$ amounts therefore to minimize the pseudo-hyperbolic distance δ between the filter's reflection parameter $S_{2,2}$ and the conjugate of the load's reflection $\overline{L_{1,1}}$, 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.

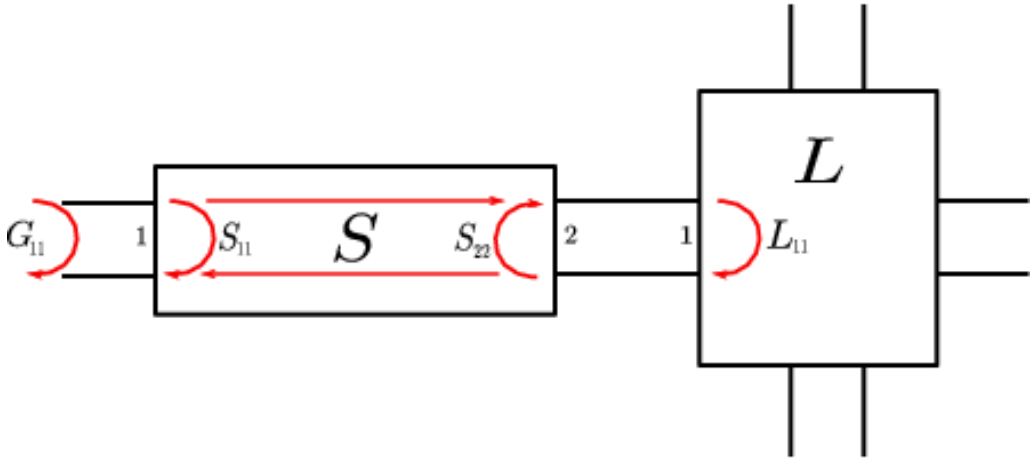


Figure 5. Filter plugged on a system with reflection coefficient L_{11}

6.2.1. Multiplexer synthesis via interpolation and common junction design

Based on our work linking Nevanlinna-Pick interpolation and point-wise matching techniques [6] we tackled the synthesis of a multiplexer on the basis of frequency specifications relative to a triplexer furnished by CNES and deemed to be problematic. Theoretical results guaranty the existence in this case, under a strict contractivity hypothesis on the common junction, of a simultaneous pointwise matching solution of all three channel filters. This result is however not constructive as it relies on Brouwer's fixed point theorem, a purely topological argument. In the context of the PhD of D. Martinez, we developed a continuation algorithm, starting from a completely decoupling junction and ending up with the manifold junction of interest. When the junction decouples all the channels, the overall matching problem results in 3 independent Nevanlinna-Pick interpolation problems as described in [6]: this yield the starting point of our continuation approach. The manifold peaks have also been identified as crucial here: these are resonances taking place in the common junction of the multiplexer, at which transmission of energy becomes impossible between a given channel and the common port. These peaks have been mathematically characterized, and a systematic combinatorial algorithm designed for the synthesis of a "peak free" manifold junction. In particular it was proven, that an extremely compact junction is needed to fit the specifications furnished by CNES: when dispersive effects increase (and they do with the size of the junction) the appearance of manifold peaks has been proven inevitable. Using a continuation approach to compute the channel filters responses and a combinatorial procedure to design a peak-free junction, a complete triplexer has been synthesized that fits the CNES specifications. The synthesis was first considered in terms of circuits and eventually transformed in a real hardware realized in waveguide technology (see Figure.6). The latter is currently being manufactured at XLIM laboratories, where our colleague S. Bila is co-advising D. Martinez' PhD.

6.2.2. Uniform matching and global optimality considerations

The interpolation procedure of [6] provides us with 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, and this for a given maximal

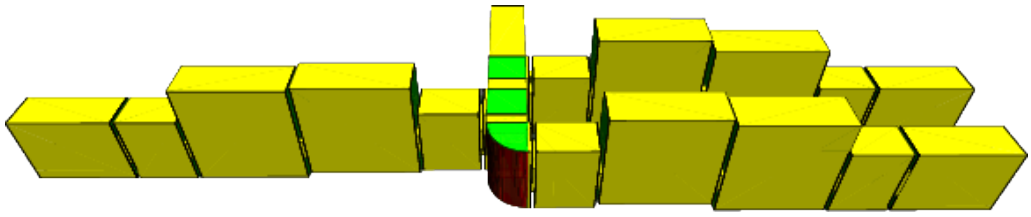


Figure 6. Full wave simulation of the realized triplexer, constituted of a very compact fishbone junction and three channel filters, each of order 6

degree n_c of the matching network. Following the approach of Fano and Youla, we considered the problem of designing a 2×2 loss-less frequency response, under the condition that a specified load can be "unchained" from one of its port. This classically amounts to set interpolation conditions on the response at the transmission zeros of the Darlington extension of the load. When the load admits a rational representation of degree $n_a = 1$, 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. When the load is of degree greater than 1, our approach is a convex relaxation of the original problem as the computed matching circuit has in general degree $n_c + n_a - 1$. This delivers lower bounds for the original matching problem, the first that are known of this problem under degree constraint.

The internal representation of our problem, relies on the use of a Pick matrix $\mathcal{P}$ depending on a positive polynomial p, that needs to be positive in terms of matrices, that is $\mathcal{P}(p) \succeq 0$. Although we know for the convexity of our global formulation [17], the concavity of the matrix valued map $\mathcal{P}$ is not evident at all. Using arguments of matrix valued Nevanlinna-Pick interpolation we were able to establish it this years, that is: for all pair of positive polynomials (p_1, p_2) the following holds,

$$\mathcal{P}(\alpha p_1 + (1-\alpha)p_2) \succeq \alpha\mathcal{P}(p_1) + (1-\alpha)\mathcal{P}(p_2).$$

This is an important result, as it justifies the use of Lagrangian relaxation for our problem that appears to be a non-linear, convex, semi-definite optimization program (NLSDP), the hardest class among current convex optimization. We plan to build on this result, in order to obtain a critical point equation to our problem, in terms of extremal points of the involved polynomials.

The software implementation developed within the PhD of D. Martinez, combining logarithmic barrier functions and Lagrangian relaxation techniques has been made available for practitioners as Matlab library called Puma 5.2 . Results obtained thank to this tool, have been presented in [15], [18] and on a dedicated workshop at the conference IMS2018. Design of use cases, for antenna matching problems relevant in 5G and IOT applications are currently being analyzed with LEAT, within the context of G. Bose's PhD.

6.3. 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. This activity has gained momentum with the doctoral work of (S. Fueyo), co-advised with J.-B. Pomet (from the McTao Inria project-team) and the postdoctoral stay of (A. Cooman) that eventually resulted in substantial software developments. Application of our work to oscillator design methodologies started recently in collaboration 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 [19].

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 [9], that we further improved in [16] to address the design of oscillators, in collaboration with Smain Amari. The evaluation of the admittance function of interest is furnished, on a finite frequency band, by a circuit simulator. Progress were made on the interpolation procedure and the determination of a filtering function that are used to obtain a functional representation of high order of the unstable part of the admittance function to be analyzed. The latter was tested on a time-delayed Chua oscillator circuit: the analytical model of this circuit is known in closed form, and using continuation techniques on the involved delay components it is possible to compute the exact unstable poles of this circuit: two being exactly at the oscillators frequency, while two others spurious poles at DC frequency are present and are usually hard to detect with classical methods. Our approximation based procedure, which was fed with incomplete frequency data estimation of the admittance, was able to recover all poles within a relative error of less than 0.01%. A real world example of an MMIC oscillator was also analyzed and confirmed the procedure's effectiveness. A complete software library called pisa (see Section 5.1) have been developed to render these techniques accessible for practitioners. Although these results are very satisfying in practice, we are aiming for a result that would link together, the width of the measurement band, the density of the measurement points with the precision with which a pole, located within a certain depth into the complex plan can be identified. Extensions of our procedure to the strong signal case, where linearization is considered around a periodic trajectory, yielding harmonic transfer functions is also being worked on.

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 showed in previous years 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. This year, we proved a similar result for general circuits, provided that they are passive at very high frequency. For this, we use Lyapunov functions for the transmission lines to establish exponential L^2-stability, and then rely on counting techniques and impulse response estimates to obtain L^∞ stability from the exponential L^2-stability. We

are currently developing the link between the monodromy operators of a general circuit and the so-called Harmonic Transfer Function of the circuit. A practical application of this result will be 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.

6.4. The Hardy-Hodge decomposition

Participant: Laurent Baratchart.

(This is joint work with T. Qian and P. Dang from the university of Macao.) It was proven in previous year that on a smooth compact hypersurface Σ 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 Σ, a harmonic gradient from outside Σ, and a tangent divergence-free field. This year we extended this result to Lipschitz surfaces for $2-\varepsilon < p < 2+\varepsilon'$, where ε and ε' depend on the Lipschitz constant of the surface. We also proved that the decomposition is valid for $1 < p < \infty$ when Σ is VMO-smooth (*i.e.*Σ is locally the graph of Lipschitz function with derivatives in VMO). By projection onto the tangent space, this gives a Helmholtz-Hodge decomposition for vector fields on a Lipschitz hypersurface, which is apparently new since existing results deal with smooth surfaces. In fact, the Helmholtz-Hodge decomposition is valid on surfaces (not just hypersurfaces), and an article is currently being written on this topic. The Hardy-Hodge decomposition generalizes the classical Plemelj formulas from complex analysis.

6.5. Imaging and modeling ancient materials

Participants: Vanna Lisa Coli, Juliette Leblond.

This is a very recent activity of the team, linked to images classification in archaeology in the framework of the project ToMaT, "Multiscale Tomography: imaging and modeling ancient materials, technical traditions and transfers" (see Section 8.1), and to the post-doctoral stay of V. L. Coli ; it is pursued in collaboration with L. Blanc-Féraud (project-team Morpheme, I3S-CNRS/Inria Sophia/iBV), D. Binder (CEPAM-CNRS, Nice), in particular.

The pottery style is classically used as the main cultural marker within Neolithic studies. Archaeological analyses focus on pottery technology, and particularly on the first stages of pottery manufacturing processes. These stages are the most demonstrative for identifying the technical traditions, as they are considered as crucial in apprenticeship processes. Until now, the identification of pottery manufacturing methods was based on macro-traces analysis, i.e. surface topography, breaks and discontinuities indicating the type of elements (coils, slabs...) and the way they were put together for building the pots. Overcoming the limitations inherent to the macroscopic pottery examination requires a complete access to the internal structure of the pots. Micro-computed tomography (μCT) has recently been used for exploring ancient materials microstructure. This non-invasive method provides quantitative data for a big set of proxies and is perfectly adapted to the analysis of Cultural heritage materials.

The main challenge of our current analyses aims to overcome the lack of existing protocols to apply in order to quantify observations. In order to characterize the manufacturing sequences, the mapping of the paste variability (distribution and composition of temper) and the discontinuities linked to different classes of pores, fabrics and/or organic inclusions appears promising. The totality of the acquired data composes a set of 2-D and 3-D surface and volume data at different resolutions and with specific physical characteristics related to each acquisition modality (multimodal and multi-scale data). Specific shape recognition methods need to be developed by application of robust imaging techniques and 3-D-shapes recognition algorithms.

In a first step, we devised a method to isolate pores from the 3-D data volumes; we are currently focusing our investigation on 2-D slices displaying pores locations and we considering several data processing treatments, such as multiresolution processing and Hough transform (derived from Radon transform), in order to evaluate their outcome when applied to these very particular images. Different possibilities of investigation will be analyzed as well, such as "a contrario" analysis and deep learning techniques.

6.6. Behavior of poles in meromorphic approximation

Participant: Laurent Baratchart.

We proved this year that if a function is holomorphic outside a disk of radius $r < 1$ in the complex plane, then its best approximant on the unit circle, in the uniform norm, by a meromorphic function having at most n poles in the unit disk has at most m poles of modulus greater than r, where m is independent of n. This is the first result on the behavior of singularities in meromorphic approximation to a function with 2-D singular set. We are currently working on analogs in a non-circular geometry and in rational rather than meromorphic approximation.

6.7. Tools for numerically guaranteed computations

Participant: Sylvain Chevillard.

The overall and long-term goal is to enhance the quality of numerical computations. The software tool Sollya (see Section 3.4.5), developed together with C. Lauter (Université Pierre et Marie Curie) intends to provide an interactive environment for performing numerically rigorous computations. It comes as a standalone tool and also as a C library that allows one to benefit from all the features of the tool in C programs.

In September 2018, we released version 7.0. Among other things, this release fixes some bugs and improves the way base functions are internally handled. Another important novelty of 2018 is that Sollya now comes with the companion `pythonsollya`[0] proposed by third-party developers to provide all the features of Sollya within Python. Some of the novelties in the API of the library version of Sollya 7.0, were made to ease the development of `pythonsollya`.

[0] https://gitlab.com/metalibm-dev/pythonsollya/

I4S Project-Team

5. New Results

5.1. System identification

5.1.1. Linear parameter varying system local model interpolation

Participant: Qinghua Zhang.

The local approach to linear parameter varying (LPV) system identification consists in interpolating a collection of linear time invariant (LTI) models, which have been estimated from data acquired at different working points of a nonlinear system. Interpolation is essential in this approach. When the local LTI models are in state-space form, as each local model can be estimated with an arbitrary state basis, it is widely acknowledged that the local models should be made coherent before their interpolation. In order to avoid the delicate task of making local state-space models coherent, a new interpolation method of local state-space models is proposed in this work, which does not require coherent local models. This method is based on the reduction of the large state-space model built by combining the local models. This work has been presented at SYSID 2018 [39].

5.1.2. State estimation for stochastic time varying systems with disturbance rejection

Participant: Qinghua Zhang.

State estimation in the presence of unknown disturbances is useful for the design of robust systems in different engineering fields. Most results available on this topic are restricted to linear time invariant (LTI) systems, whereas linear time varying (LTV) systems have been studied to a lesser extent. Existing results on LTV systems are mainly based on the minimization of the state estimation error covariance, ignoring the important issue of the stability of the state estimation error dynamics, which has been a main focus of the studies in the LTI case. The purpose of this work is to propose a numerically efficient algorithm for state estimation with disturbance rejection, in the general framework of LTV stochastic systems, including linear parameter varying (LPV) systems, with easily checkable conditions guaranteeing the stability of the algorithm. The design method is conceptually simple: disturbance is first rejected from the state equation by appropriate output injection, then the Kalman filter is applied to the resulting state-space model after the output injection. This work has been carried out in collaboration with Beijing University of Posts and Telecommunications (China) and has been presented at SYSID 2018 [40].

5.1.3. Variance estimation of modal indicators from subspace-based system identification

Participants: Michael Doehler, Laurent Mevel.

This work has been carried out in collaboration with Szymon Gres at Aalborg University and Palle Andersen at SVS.

One of the other practical modal indicators is Modal Assurance Criterion (MAC), for which uncertainty computation scheme is missing. This paper builds on the previous results using the propagation of the measurement uncertainties to estimates of MAC. The sensitivity of the MAC with respect to output covariances is derived using a first order perturbations and the uncertainties are propagated using the Delta method. The influence of the underlying mode shape scaling on both the uncertainty of mode shapes and MAC is investigated [22].

5.1.4. On damage detection system information for structural systems

5.1.4.1. On damage detection system information for structural systems

Participant: Michael Doehler.

Damage detection systems (DDSs) provide information on the integrity of structural systems in contrast to local information from inspections or non-destructive testing (NDT) techniques. In this paper, an approach is developed that utilizes DDS information to update structural system reliability and integrate this information into risk and decision analyses. For updating of the structural system reliability, an approach is developed based on Bayesian updating facilitating the use of DDS information on structural system level and thus for a structural system risk analysis. The structural system risk analysis encompasses the static, dynamic, deterioration, reliability and consequence models, which provide the basis for calculating the direct risks due to component failure and the indirect risks due to system failure[16].

5.1.4.2. The effects of deterioration models on the value of damage detection information
Participant: Michael Doehler.

This paper addresses the effects of the deterioration on the value of damage detection information. The quantification of the value of damage detection information for deteriorated structures is based on Bayesian pre-posterior decision analysis, comprising structural system performance models, consequence, benefit and costs models and damage detection information models throughout the service life of a structural system. With the developed approach, the value of damage detection information for a statically determinate Pratt truss bridge girder subjected to different deterioration models is calculated. The analysis shows the impact of the deterioration model parameters on the value of damage detection information. [28].

5.1.4.3. The effects of SHM system parameters on the value of damage detection information
Participant: Michael Doehler.

This paper addresses how the value of damage detection information depends on key parameters of the Structural Health Monitoring (SHM) system including number of sensors and sensor locations. The quantification of the value of information (VoI) is an expected utility based Bayesian decision analysis method for quantifying the difference of the expected economic benefits with and without information. The (pre-)posterior probability is computed utilizing the Bayesian updating theorem for all possible indications. Through the analysis of the value of information with different SHM system characteristics, the settings of DDS can be optimized for minimum expected costs and risks before implementation [29].

5.1.5. Filtering approaches for damage detection

5.1.5.1. Adaptive Kalman filter for actuator fault diagnosis
Participant: Qinghua Zhang.

An adaptive Kalman filter is proposed in this work for actuator fault diagnosis in discrete time stochastic time varying systems. By modeling actuator faults as parameter changes, fault diagnosis is performed through joint state-parameter estimation in the considered stochastic framework. Under the classical uniform complete observability-controllability conditions and a persistent excitation condition, the exponential stability of the proposed adaptive Kalman filter is rigorously analyzed. In addition to the minimum variance property of the combined state and parameter estimation errors, it is shown that the parameter estimation within the proposed adaptive Kalman filter is equivalent to the recursive least squares algorithm formulated for a fictive regression problem. These results have been published in [17].

5.1.5.2. Zonotopic state estimation and fault detection for systems with both time-varing and time-invariant uncertainties
Participant: Qinghua Zhang.

This paper proposes a robust guaranteed state estimation method with application to fault detection by combining H_∞ observer design with zonotopic analysis for discrete-time systems with both time-varing and time-invariant uncertainties. In order to improve the estimation accuracy, based on the H_∞ technique, the observer design is achieved by solving a linear matrix inequality. The main contribution of this paper lies in that the time invariance of some uncertainties is considered to reduce the conservatism of interval estimation. This work has been carried out in collaboration with Harbin Institute of Technology (China) and with Universitat Politècnica de Catalunya (Spain), and has been presented at SAFEPROCESS 2018 [37].

5.1.5.3. Local adaptive observers for time-varying systems with parameter-dependent state matrices
Participant: Qinghua Zhang.

The purpose of this work is to design an adaptive observer for linear time-varying systems whose state matrix is affine in some unknown parameters. In this case, the proposed observer generates state and parameter estimates, which exponentially converge to the plant state and the true parameters, respectively. The results are then extended to systems whose state matrix is nonlinear, instead of being affine, in the unknown parameters. This work has been carried out in collaboration with Université de Lorraine-CNRS-CRAN and has been presented at CDC 2018 [45].

5.1.5.4. Seismic-induced damage detection through parallel force and parameter estimation using an improved interacting Particle-Kalman filter

Standard filtering techniques for structural parameter estimation assume that the input force is either known 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. In this paper, the input force is considered to be an additional state that is estimated in parallel to the structural parameters. Two concurrent filters are employed for parameters and force respectively. For the parameters, an interacting Particle-Kalman filter is used to target systems with correlated noise. Alongside this, a second filter is used to estimate the seismic force acting on the structure [15].

5.1.5.5. Bayesian parameter estimation for parameter varying systems using interacting Kalman filters
Participants: Antoine Crinière, Laurent Mevel, Jean Dumoulin.

Existing filtering based structural health monitoring (SHM) algorithms assume constant noise environment which does not always conform to the reality as noise is hardly stationary. Thus to ensure optimal solution even with non-stationary noise processes, the assumed statistical noise models have to be updated periodically. This work incorporates a modification in the existing Interacting Particle-Kalman Filter (IPKF) to enhance its detection capability in presence of non-stationary noise processes. The Kalman filters (KF) within the IPKF have been replaced with a maximum Correntropy criterion (MCC) based KF that, unlike regular KF, takes moments beyond second order into consideration [32].

5.1.6. Damage localization for mechanical structures

5.1.6.1. Damage localization using the stochastic load vectors
Participants: Laurent Mevel, Michael Doehler.

This work was done in collaboration with BAM (Berlin) and GEM (Nantes).

In this work, a benchmark application is proposed, namely a 1/200 scale model of the Saint-Nazaire Bridge, which is a cable-stayed bridge spanning the Loire River near the river's mouth. The region of interest, the central metallic structure, measures 720 meters. The aim of the instrumentation is to assess the capability of damage assessment methods to assess a cable failure. The model is instrumented with ten accelerometers and excited by white noise. A damage localization method is applied to test the proposed setup, namely the statistical damage locating vector approach (S-SDDLV). With this method, vibration measurements from the (healthy) reference and damaged states of the structure are confronted to a finite element of the reference state. Damage indicators are provided for the different structural elements that are easy to compute, without updating the model parameters, and taking into account the intrinsic uncertainty of noisy measurements. [21].

5.1.6.2. Asymptotic analysis of subspace-based data-driven residual for fault detection with uncertain reference
Participants: Laurent Mevel, Michael Doehler, Eva Viefhues.

This work was in collaboration with BAM (Berlin).

The local asymptotic approach is promising for vibration-based fault diagnosis when associated to a subspace-based residual function and efficient hypothesis testing tools. In the residual function, the left null space of the observability matrix associated to a reference model is confronted to the Hankel matrix of output covariances estimated from test data. When this left null space is not perfectly known from a model, it should be replaced by an estimate from data to avoid model errors in the residual computation. In this paper, the asymptotic distribution of the resulting data-driven residual is analyzed and its covariance is estimated, which includes also the covariance related to the reference null space estimate [36].

5.1.7. Smarts roads and R5G

5.1.7.1. Multi-physics models for Energy Harvesting performance evaluation

Participants: Jean Dumoulin, Nicolas Le Touz.

We present in this paper the concept of solar hybrid road and focus on the thermal performances of such system. A finite element model is presented to couple thermal diffusion, hydraulic convection and radiative transfer. This numerical model allows to compute the temperature field for different weather conditions and also to evaluate the thermal performances of the system. Annual simulations are performed and a comparison between two surface layer solutions for different locations and climates is presented and discussed[23].

5.1.7.2. Optimal command for defreezing of solar road

Participants: Jean Dumoulin, Nicolas Le Touz.

The study presented in [26] aims to optimize the amount of energy to bring to a hybrid solar road to prevent the formation of ice on the surface. The optimal control law studied is based on a finite element multiphysics model, developed to compute the temperature field in the structure under varying environmental conditions presented in [25]. A penalization of freezing periods at the surface is introduced and the energy to be supplied to the system to preserve it is calculated from the adjoint state method [24].

5.1.8. Infrared Thermography

5.1.8.1. Sensitivity of infrared camera to environmental parameters

Participants: Laurent Mevel, Jean Dumoulin, Thibaud Toullier.

The purpose of this study is to characterize the influence of environmental parameters for long-term in-situ structure monitoring as well as projections errors due to camera view and digitization. The model used to convert 3 year gathered data to temperature is firstly presented and discussed. Then, the effect of camera resectioning on infrared measurements is commented. Finally, the effect of the environmental parameters is studied and perspectives are proposed [35].

5.1.8.2. Joint Estimation of emissivity and temeperature

Participants: Laurent Mevel, Jean Dumoulin, Thibaud Toullier.

This study deals with the simultaneous assessment of emissivity and surface temperature. of objects observed by in-situ infrared thermography. Temperature measurement by thermography infrared is hampered by the lack of knowledge of the radiative properties of the real world. The light received from a target by an infrared camera is estimated by the method of progressive radiosities implemented on a map graphic in order evaluate the sensitivity of four methods of separation of emissivity and temperature [34].

5.1.9. Sensor and hardware based research

5.1.9.1. Reflectometry

Participant: Qinghua Zhang.

5.1.9.2. De-embedding unmatched connectors for electric cable fault diagnosis

Participant: Qinghua Zhang.

In order to make accurate reflectometry measurements on electric cables for fault diagnosis, connector de-embedding is a procedure for compensating measurement distortions caused by unmatched connectors. The key step in such a procedure is the characterization of the connectors, which is realized through measurements on a pair of connectors linked by a short cable segment. The analysis for deducing the characteristics of a single connector from measurements made on an assembled pair is known as the bisection problem. In this paper, after recalling the underdetermined nature of the bisection problem, a practically effective de-embedding procedure is proposed based on a particular regularization technique. This work has been carried out in collaboration with EDF R&D and has been presented at SAFEPROCESS 2018 [38].

5.1.9.3. Active Infrared thermography by robot

Participants: Jean Dumoulin, Ludovic Gaverina.

In this paper, two Non Destructive Testing approaches by active infrared thermography mounted on a 6-axis robot are presented and studied. An automated procedure is proposed to reconstruct thermal image sequences issued from the two scanning procedure studied: Line Scan and Flying Line procedures. Defective area detection is performed by image processing and an inverse technique based on thermal quadrupole method is used to map the depth of flaws [31].

5.1.9.4. Shunting monitoring in railway track circuit receivers

Participant: Vincent Le Cam.

Track circuits play a major role in railway signaling. In some exceptional conditions, poor rail/wheel contact conditions may lead to a non-detection of the train on the zone. The paper presents new detection approaches based on signal processing on an experiment with a dedicated train running on a track equipped with a track circuit. The second objective is to present a strategy to test new detection criteria on commercial zones over a long period of time using PEGASE [30].

MCTAO Project-Team

7. New Results

7.1. Well posedness in Optimal Transport

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

Concerning the Kantorovitch problem, in continuation of the work by McCann and Rifford [67], Moameni and Rifford have studied (see [12]) 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.

Concerning the Monge problem in the sub-Riemannian setting, Zeinab Badreddine [2] obtained the first result of well-posedness in cases where singular minimizing curves may be present. This study is related to the so-called measure contraction property. In collaboration with Rifford [22], Badreddine obtained new classes of sub-Riemannian structures satisfying measure contraction properties.

7.2. Strong Sard conjecture for sub-Riemannian structures

Participants: Ludovic Rifford, André Belotto Da Silva [Université Aix-Marseille, France], Alessio Figalli [ETH, Swizerland], Adam Parusinski [Université Côte d'Azur, France].

In [25], we address the strong Sard conjecture for sub-Riemannian structures on 3-dimensional analytic manifolds. More precisely, given a totally non-holonomic analytic distribution of rank 2 on a 3-dimensional analytic manifold, we investigate the size of the set of points that can be reached by singular horizontal paths starting from a given point and prove that it has Hausdorff dimension at most 1. In fact, this set is a semi-analytic curve, provided that the lengths of the singular curves under consideration are bounded with respect to a given complete Riemannian metric. As a consequence, combining these techniques with recent developments on the regularity of sub-Riemannian minimizing geodesics, we prove that minimizing sub-Riemannian geodesics in 3-dimensional analytic manifolds are always of class C1, and actually are analytic outside of a finite set of points. This paper can be seen as a major step toward a proof of the Sard conjecture in any dimension.

This is a drastic improvement of the results published in [4] (appeared this year), that proved a slightly weaker property for a less general class of systems.

7.3. Optimal approximation of internal controls for a wave-type problem with fractional Laplacian using finite-difference method

Participants: Pierre Lissy, Ionel Roventa [University of Craiova, Romania].

In paper [30], a finite-difference semi-discrete scheme for the approximation of internal controls of a one-dimensional evolution problem of hyperbolic type involving the spectral fractional Laplacian is considered. The continuous problem is controllable in arbitrary small time. However, the high frequency numerical spurious oscillations lead to a loss of the uniform (with respect to the mesh size) controllability property of the semi-discrete model in the natural setting. For all initial data in the natural energy space, if we filter the high frequencies of these initial data in an optimal way, the uniform controllability property in arbitrary small time is restored. The proof is mainly based on a (non-classic) moment method.

7.4. Singularities in minimum time control

Participants: Jean-Baptiste Caillau, Michaël Orieux, Jacques Féjoz [Univ. Paris Dauphine], Robert Roussarie [Univ. Bourgogne-Franche Comté].

We analyze singularities arising in minimum time systems. Consider a control affine system in dimension four with control on the disc such that the controlled fields together with their first order Lie brackets with the drift have full rank. There is a natural stratification of the codimension two singular set in the cotangent bundle leading to a local classification of extremals in terms of singular and bang arcs. This analysis was done in [56] using the nilpotent model, and extended in [35] by interpreting the singularities of the extremal flow as equilibrium points of a regularized dynamics to prove the continuity of the flow. After a suitable blow-up, one can actually treat these singularities as connections of pairs of normally hyperbolic invariant manifolds in order to find a suitable stratification of the flow and prove finer regularity properties. Another issue is to be able to give global bounds on the number of these heteroclinic connections. This can be done by means of *à la Sturm* estimations. This work is part of the PhD thesis of Michaël Orieux [1] and is described in the preprint [28]. In an ongoing work, we also investigate second order sufficient conditions for extremals with such singularities.

7.5. Software advances

Participants: Jean-Baptiste Caillau, Olivier Cots [Univ. Toulouse], Lamberto Dell'Elce, Thibaud Kloczko, Pierre Martinon [COMMANDS team], Jean-Baptiste Pomet.

McTAO and COMMANDS have been awarded an AMDT (Action Mutualisée de DéveloppemenT) funding of two years to develop a common interface for *Hampath* and BOCOP. This AMDT, coined `ct` for "Control tools" is to start in January 2019. Our midterm goal is to set the standard for the numerical resolution of optimal control problems. On the basis of the two well established codes BOCOP and *Hampath* from the optimal control community, thanks to this ADT we want to design a high-level modular architecture in order to:

- interoperate BOCOP and *Hampath*,
- offer a high-level common user interface for the two codes.

Another expected outcome of the ADT is to integrate state of the art processes into the development of the two solvers (collaborative dev tools, reliable repositories, continuous integration...)

7.6. Averaging optimal control problems with two frequencies

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

Averaging is a valuable technique to gain understanding in the long-term evolution of fast-oscillating dynamical systems. Recent contributions (pioneered by McTAO members in the framework of a long-standing project funded by CNES and Thales Alenia Space) proved that averaging can be applied to the extremal flow of optimal control problems. This study extends the aforementioned results by tackling averaging of time optimal systems with two fast variables with particular emphasis on the treatment of adjoint variables and on the understanding of resonance effects on their dynamics. The chapter [18] details part of this work, and a dedicated paper is in preparation [29].

7.7. Integrability properties of the controlled Kepler problem

Participants: Jean-Baptiste Caillau, Michaël Orieux, Jacques Féjoz [Univ. Paris Dauphine], Robert Roussarie [Univ. Bourgogne-Franche Comté].

We prove, using Moralès–Ramis theorem, that the minimum-time controlled Kepler problem is not meromorphically integrable in the Liouville sense on the Riemann surface of its Hamiltonian. The Kepler problem is a classical reduction of the two-body problem. We think of the Cartesian coordinate as being the position of a spacecraft, and of the attraction as the action of the Earth. We are interested in controlling the transfer of the spacecraft from one Keplerian orbit towards another one, in the plane. By virtue of Pontrjagin maximum principle, the minimum time dynamics is a Hamiltonian system. The controlled Kepler problem can be embedded in the two parameter family obtained when considering the control of the circular restricted three-body

problem. In the uncontrolled model, it is well known that the Kepler case is integrable and geodesic (there exists a Riemannian metric such that Keplerian curves are geodesics of this metric), while there are obstructions to integrability for positive ratio of masses. In the controlled case, the Kepler problem for the energy cost has been shown to be integrable (and geodesic) when suitably averaged. The aim of this work is to study the integrability properties of the Kepler problem for time minimization. The pioneering work of Ziglin in the 80s, followed by the modern formulation of differential Galois theory in the late 90s by Moralès, Ramis and Simó, have led to a very diverse literature on the integrability of Hamiltonian systems. According to Pontrjagin Maximum principle, one can turn general optimization problems with dynamical constraints into Hamiltonian systems, which are generally not everywhere differentiable. Optimal control theory thus provides an abundant class of dynamical systems for which integrability is a central question. Yet, differential Galois theory has not so often been applied in this context, in part because of the difficulty brought by the singularities. Notwithstanding theses singularities, we show how to apply these ideas to the Kepler system, and prove that it is not meromorphically integrable in the Liouville sense on the Riemann surface of its Hamiltonian. This work is also part of the PhD thesis of Michaël Orieux [1] and is described in the paper [11].

7.8. Quasi-satellite orbits in the proximity of Martian moons

Participants: Lamberto Dell'Elce, Nicola Baresi [JAXA, Japan], Josué Cardoso Dos Santos [Sao Paolo State University, Brasil], Yasuhiro Kawakatsu [JAXA, Japan].

The Martian Moons eXploration mission is currently under development at the Japan space agency (JAXA) and will be the first spacecraft mission to retrieve pristine samples from the surface of Phobos. In preparation for the sampling operations, MMX will collect observations of Phobos from stable retrograde relative trajectories, which are referred to as quasi-satellite orbits (QSOs). This study investigates the navigability of mid- and high-altitude QSOs in terms of relative orbit elements. After developing an analytical model for the long-term evolution of QSOs and a numerical map between mean and osculating (instantaneous) orbital elements, we use a Lyapunov control law for orbit maintenance purposes based on mean relative orbit element differences. These results were presented in [16] and they pave the way for a perspective collaboration between JAXA and McTAO.

7.9. The Copepod and Purcel swimmer

Participants: Bernard Bonnard, Jérémy Rouot, Piernicola Bettiol, Monique Chyba [U. Hawaii].

In the continuation to J. Rouot Phd thesis (2016), our results are presented in a series of papers [7], [5], [6]. The most efficient strokes are computed using geometric studies and numerical simulations, in relation with sub-Riemannian geometry and periodic optimal control algorithms. In the copepod case the model is validated by simulations and a copepod robot was constructed at Hawaii to mimic the copepod. The experiment was reproduced at EPF Troyes under the supervision of J. Rouot. The reference [21] gathers the results of MRI and swimmers in a unified setting combining geometric and numeric techniques developed in McTAO.

7.10. Multi-link vs flexible filament swimmers

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

The inertialess fluid-structure interactions of active or passive inextensible filaments and slender-rods are ubiquitous in nature, from the dynamics of semi-flexible polymers and cytoskeletal filaments to cellular mechanics and flagella, or in artificial micro-swimmers (see Section 7.12).

For a microscopic inextensible elastic filament immersed into a fluid, even approximating the fluid-structure interaction by the Resistive Force Theory formulation, the system of PDEs resulting from elastohydrodynamical laws is structurally convoluted and demanding numerically. The N-link swimmer model, where the continuous filament is replaced by N segments with elasticity concentrated at the joints, can be seen as a coarse-graining formulation of the latter. In [10] (see also [31]), the N-link swimmer model is presented in this perspetive and it is demonstrated numerically how this system can be used as an alternative. It can be solved numerically with any ODE solver and overcomes well-known numerical instabilities when solving numerically the full PDE for the filament. Computations can be as much as a hundred times faster. Generalisations for more complex interactions are demonstrated on four examples commonly found in biological systems, a Matlab code is provided as a basis for further generalisations.

More theoretical study of this approximation property are under investigation, also in the framework of Clément Moreau's PhD.

7.11. Energy-optimal strokes for multi-link micro-swimmers

Participants: Laetitia Giraldi, François Alouges [École Polytechnique], Antonio Desimone [SISSA Trieste, Italy], Yshar Or [Technion, Haifa, Israel], Oren Wiezel [Technion, Haifa, Israel].

In a common work that is presented in [33], submitted to *New Journal of Physics*, we consider a slender planar multi-link micro-swimmer (N links, see Section 7.10), where the time derivatives of the angles defining the shape are taken as controls, and we are mostly interested in small-amplitude undulations about its straight configuration.

Based only on the leading order dynamics in that vicinity, the optimal stroke to achieve a given prescribed displacement in a given time period is then obtained as the largest eigenvalue solution of a constrained optimal control problem. Remarkably, the optimal stroke is an ellipse lying within a two-dimensional plane in the (N-1)-dimensional space of joint angles, where N can be arbitrarily large. For large N, the optimal stroke is a traveling wave of bending, modulo edge effects.

We also solved, numerically, the fully non-linear optimal control problem for the cases $N = 3$ (Purcell's three-link swimmer) and $N = 5$ showing that, as the prescribed displacement becomes small, the optimal solutions obtained using the small-amplitude assumption are recovered. We also show that, when the prescribed displacements become large, the picture is different. For $N = 3$ we recover the non-convex planar loops already known from previous studies. For $N = 5$ we obtain non-planar loops, raising the question of characterizing the geometry of complex high-dimensional loops.

7.12. Swimming magnetic micro-robots

Participants: Luca Berti, Yacine El Alaoui-Faris, Laetitia Giraldi, Jean-Baptiste Pomet, Christophe Prud'Homme [Université de Strasbourg], Stéphane Régnier [UPMC - Sorbonne Universités].

We are in a collaboration with the Parisian robotics laboratory ISIR (Institut des Systèmes Intelligents et de Robotique) to enhance the control of artificial micro-swimmers that are actually built and implemented there. This involves building models and using them for control design. These robots are "magnetic micro-swimmers": part of them is magnetized and the control is an ambient magnetic field.

Yacine El Alaoui-Faris's PhD, co-advised with Stéphane Régnier, started October, 2017. It is centered on finite-dimensional models. The robots under consideration are made of a magnetic head and a flexible tail; the model is a 3-D counterpart of the planar "multi-link micro-swimmers" discussed in Section 7.10 .

The validation of this nonlinear ODE model, with or without magnetic actuation, has been achieved this year, both against continuous models present in the literature and against experimental data at ISIR. This model has a definite interest by itself, and in the case of magnetic actuation, it allowed the numerical computation of periodic controls (magnetic field) that optimize the longitudinal velocity with prescribed maximum amplitude of the magnetic field oscillations. This process is described in a manuscript under preparation, to be submitted to *Physical Review Letters*.

These controls have very recently been tested in lab and a very significant efficiency gain over classical sinusoidal oscillations has been evidenced. This is a very encouraging experimental result.

Luca Berti's PhD, co-advised with Christophe Prud'homme, started this fall. It is focused on PDE models that are closer to the real physics but more intricate. His master's thesis was mostly a numerical project in the framework of Cemracs 2018 (http://smai.emath.fr/cemracs/cemracs18/), where we modeled the displacement of a deformable swimmer using a coupling between Stokes equations and hyper-elasticity equations. The PDEs was solved using the Feel++ finite elements library. We validated the fluid model using an exact solution for a rotating rigid body. The motion of a one-hinged swimmer (which obeys to the scallop theorem) was successfully simulated. The physical robots from ISIR are now considered in his PhD.

7.13. Necessary conditions for local controllability, motivated by the Two-link Magneto-elastic Micro-swimmer

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

After proving in [66] a local controllability for the 2-link magneto-elastic swimmer around its straight configuration and noting that this property is weaker than Small-Time Locally Controllable (STLC), we investigated "full" STLC for this system, and were able to show that, except for very specific values of the lengths and magnetizations, this system is *not* STLC. This is published in [9]. This lead us to necessary condition for STLC for more general classes of systems. This is part of Clément Moreau's doctoral research and a publication is under preparation, for classes of control-affine systems with two controls that are not micro-swimmer models, but stem from the observations in [9] and [66].

7.14. Numerical and Symbolic computations in MRI

Participants: Bernard Bonnard, Jérémy Rouot, Thibaut Verron, Olivier Cots [ENSEEIHT Toulouse].

Academic year 2016-17 with the two Postdoctoral position at Toulouse (J. Rouot at LAAS and T. Verron, Enseeith) was the opportunity to complete our investigations about the contrast and multi-saturation problem in MRI. This concerns numeric and symbolic computations using Hampath, Bocop, Gloptipoly and Maple software. The reference [27], to be published in MCRF, contains all the results and techniques about this project and is the final paper of this longstanding work in quantum theory.

7.15. Stability of nonlinear high frequency amplifiers

Participants: Laurent Baratchart [FACTAS project-team], Sébastien Fueyo, Jean-Baptiste Pomet, Gilles Lebeau.

Sébastien Fueyo's PhD is co-advised on this topic. The problem is presented in Section 4.4 .

These amplifiers contain on the one hand nonlinear active components and on the other hand lines, that induce some sort of delays and make the system infinite-dimensional: they are, for each choice of a periodic input, a nonlinear infinite dimensional dynamical system. The Computer Aided Design tools mentioned in Section 4.4 provide a periodic solution under this periodic forcing and may also give the frequency response of the linearized system along this trajectory with some artificial "small" excitation. The goal is to deduce stability from these data.

It is an opportunity to build theoretical basis and justification to a stability analysis through harmonic identification; the latter is one of the specialties of FACTAS, we collaborate on the infinite-dimensional nonlinear stability analysis for periodic solutions and how it works with the results of harmonic identification.

On academic examples of simple circuits, we have given full justification (with some possible obstructions) to the prediction of stability through transfer function identification. The theoretical interest is that the spectrum of the operator that gives stability is not as elementary as predicted in the literature, but stability can be predicted nonetheless. This was presented at a local conference, Université Côte d'Azur Complex Days in January, and a more complete publication is under preparation.

On more general structures, new results are available too, publications are in progress.

7.16. Optimal sampled-control with applications to Muscular Control

Participants: Bernard Bonnard, Toufik Bakir [L2I, Univ. de Bourgogne Franche Conté], Jérémy Rouot.

The study was initialized two years ago under the impulse of Toufik Bakir (LE2I-UBFC). Based on preliminary experimental studies, the chosen model to muscular control integrates the fatigue variables and is known as *Ding et al force-fatigue model* in the literature. It is a refinement of the historical Hill model (Medecine Nobel Prize 1922). Preliminary results lead to construct a nonlinear observer and the optimized pulses trains are computed using MPC methods [15]. More recently in collaboration with L. Bourdin (Limoges), optimal control techniques were introduced in the framework of sampled-control problems. Pontryagin type necessary conditions were obtained with preliminary numerical simulations. On these topics, paper [23] has been submitted to *JOTA*, October 2018; [3] is accepted for publication in *Networks and Heterogeneous Media*, 2018.

7.17. An Optimal Control Strategy Separating Two Species of Microalgae in Photobioreactors

Participants: Olivier Bernard [BIOCORE project-team], Walid Djema, Laetitia Giraldi.

We investigate a minimum time control problem in a chemostat continuous photobioreactor model that describes the dynamics of two distinct microalgae populations. Our objective is to optimize the time of selection – or separation – between two species of microalgae. In [17], we focus on Droop's model which takes into account the internal quota storage of each microalgae species. Using the Pontryagin's principle, we find a dilution-based control strategy that steers the model trajectories to a suitable target in minimal time. Our study reveals that singular arcs play a key role in the optimal synthesis. Using numerical simulations, we show that the optimal control strategy is mainly of type bang-singular. A numerical optimal synthesis is performed throughout the paper, thereby confirming the optimality of the provided feedback-control law.

NECS Project-Team

7. New Results

7.1. Network systems: modeling, analysis, and estimation

7.1.1. 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. These results are presented in [57] and in [31]. We also developed an application to the control of epidemics [58].

7.1.2. Cyber-Physical Systems: a control-theoretic approach to privacy and security

Participants: F. Garin [Contact person], A. Kibangou, S. Gracy.

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, we obtain two kinds of results (see [24], [25] and the PhD thesis of S. Gracy): structural results, true for almost all interaction weights, and strongly structural results, true for all non-zero interaction weights. We consider both the case where the system graph is time-invariant, and the case where it varies in time.

When the conditions for ISO are satisfied, one can run algorithms in the same vein as a Kalman filter, in order to reconstruct the state and the unknown input from noisy measurements. These algorithms are known for the case where the input can be reconstructed with only one time-step of delay with respect to the measurements; in [54] we propose a (suboptimal) filter for the case when this is not possible, i.e., more measurements are needed for the input reconstruction.

7.1.3. Heterogeneity and uncertainty in distributed estimation from relative measurements

Participants: C. Ravazzi, N. K. Chan, P. Frasca [Contact person].

This work, presented in [34], has studied the problem of estimation from relative measurements in a graph, in which a vector indexed over the nodes has to be reconstructed from pairwise measurements of differences between its components associated to nodes connected by an edge. In order to model heterogeneity and uncertainty of the measurements, we assume them to be affected by additive noise distributed according to a Gaussian mixture. In this original setup, we formulate the problem of computing the Maximum-Likelihood (ML) estimates and we design two novel algorithms, based on Least Squares regression and Expectation-Maximization (EM). The first algorithm (LSEM) is centralized and performs the estimation from relative measurements, the soft classification of the measurements, and the estimation of the noise parameters. The second algorithm (Distributed LS-EM) is distributed and performs estimation and soft classification of the measurements, but requires the knowledge of the noise parameters. We provide rigorous proofs of convergence for both algorithms and we present numerical experiments to evaluate their performance and compare it with solutions from the literature. The experiments show the robustness of the proposed methods against different kinds of noise and, for the Distributed LS-EM, against errors in the knowledge of noise parameters.

7.1.4. Average state estimation in large-scale multi-cluster networks

Participants: U. Niazi, A. Kibangou, C. Canudas de Wit [Contact person].

In the context of the ERC project, we are addressing the problem of estimation of a functional of non-observed states. Indeed, large-scale network systems can be unobservable from the dedicated state measurements at few nodes. By resorting to an aggregation of multiple clusters of unmeasured nodes, we are investigating the observability and detectability of average states of the clusters. The approach is to obtain a reduced network system whose state vector contains the average states of the clusters. The notion of average observability is defined with respect to the observability of this reduced network system. For average observability, we have stated a necessary condition and a sufficient condition depending solely on the structure of the network. Average detectability, which is a milder notion than average observability, is also studied and a sufficient condition, under which an open-loop average state observer converges, is provided. This condition requires clusters of unmeasured nodes to have negatively balanced local outflow centrality.

7.2. Control of multi-agent systems and opinion dynamics

7.2.1. Open multi-agent systems: Dynamic consensus

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

In [53] we investigate a dynamic consensus problem for an open multi-agent system. Open multi-agent systems are characterized by a time-varying set of agents connected by a network: agents may leave and new agents may join the network at any time, thus the term “open”. The dynamic consensus problem consists in achieving agreement about the time-varying average of a set of reference signals that are assumed to be the agents’ inputs. Dynamic consensus has recently found application in the context of distributed estimation for electric demand-side management, where a large population of connected domestic appliances needs to estimate its future average power consumption. Since the considered network of devices changes as new appliances log in and out, there is a need to develop and characterize dynamic consensus algorithms for these open scenarios. In this paper we give several initial contributions both to a general theory of open multi-agent systems and to the specific problem of dynamic consensus within this context. On the theoretical side, we propose a formal definition of open multi-agent system, a suitable notion of stability, and some sufficient conditions to establish it. On the applied side, we design a novel dynamic consensus algorithm, the Open Proportional Dynamic Consensus algorithm. We characterize some of its convergence properties in the proposed open-multi-agent systems framework and we illustrate its evolution by numerical simulations.

7.2.2. Robust 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 the last four years, we have devised some possible ways to compensate for the errors caused by packet collisions, by modifying the updating weights. Since these modifications may result in a reduced convergence speed, a gain parameter is used to increase the convergence speed, and an analysis of the stability of the network is performed, leading to a criterion to choose such gain to guarantee network stability. For the implementation of the compensation method, we propose a new communication algorithm, which uses both synchronous and asynchronous mechanisms to achieve average consensus and to deal with uncertainty in packet delivery. The paper [14] provides a complete account of our results.

7.2.3. *Asynchronous opinion dynamics on the k-nearest-neighbors graph*

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

This work is about a new model of opinion dynamics with opinion-dependent connectivity. We assume that agents update their opinions asynchronously and that each agent's new opinion depends on the opinions of the k agents that are closest to it. In the paper [63], we show that the resulting dynamics is substantially different from comparable models in the literature, such as bounded-confidence models. We study the equilibria of the dynamics, observing that they are robust to perturbations caused by the introduction of new agents. We also prove that if the number of agents n is smaller than 2k, the dynamics converge to consensus. This condition is only sufficient.

7.2.4. *Quantization effects in opinion dynamics*

Participants: F. Ceragioli, P. Frasca [Contact person].

This work deals with continuous-time opinion dynamics that feature the interplay of continuous opinions and discrete behaviors. In our model, the opinion of one individual is only influenced by the behaviors of fellow individuals. The key technical difficulty in the study of these dynamics is that the right-hand sides of the equations are discontinuous and thus their solutions must be intended in some generalized sense: in our analysis, we consider both Carathéodory and Krasovskii solutions. We first prove the existence and completeness of Carathéodory solutions from every initial condition and we highlight a pathological behavior of Carathéodory solutions, which can converge to points that are not (Carathéodory) equilibria. Notably, such points can be arbitrarily far from consensus and indeed simulations show that convergence to nonconsensus configurations is common. In order to cope with these pathological attractors, we study Krasovskii solutions. We give an estimate of the asymptotic distance of all Krasovskii solutions from consensus and we prove its tightness by an example of equilibrium such that this distance is quadratic in the number of agents. This fact implies that quantization can drastically destroy consensus. However, consensus is guaranteed in some special cases, for instance, when the communication among the individuals is described by either a complete or a complete bipartite graph. These results are reported in details in [19], whereas the book chapter [66] puts them in the broader context of consensus-seeking dynamics with discontinuous right-hand side.

7.2.5. *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, but its convergence guarantees were limited to trees and regular graphs. In [36], we prove that the algorithm converges on general graphs. In [64], we offer two additional contributions to its study. We evaluate how the presence of communities in the network impacts the algorithm performance, and how the algorithm performs on networks which change topology during the execution of the algorithm.

7.2.6. *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 focus of this thesis is on the complexity of the best response algorithm to find a Nash equilibrium for potential games. Best response is a simple greedy algorithm, known to converge to a Nash equilibrium if players play one after the other in a round-robin way, but with a worst-case complexity which is exponential in the number of players. We consider instead its average complexity over the ensemble of random potential games, showing that such average complexity is surprisingly low, only linear in the number of players. Then we focus on removing the need of a centralised scheduler enforcing the round robin order of play. In [52], [21] we consider agents activated according to independent local Poisson clocks, and we show that (despite the possible overlaps of the computations of some players), we can still obtain convergence, with an average complexity of order $n \log n / \log \log n$, where n is the number of players. In [51] we 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.

7.2.7. Control of switched interconnected large-scale systems

Participants: H. Fourati [Contact person], D. Belkhiat, D. Jabri.

We proposed in [27] a new design of a decentralized output-feedback tracking control for a class of switched large-scale systems with external bounded disturbances. The controller proposed herein is synthesized to satisfy the robust H_∞ tracking performance with local disturbance attenuation levels. Based on multiple switched Lyapunov functions, sufficient conditions proving the existence of the proposed controller are formulated in terms of Linear Matrix Inequalities (LMI).

7.3. Transportation networks and vehicular systems

7.3.1. Density and flow reconstruction in urban traffic networks

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

In [56], we consider 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 characterized by a piecewise linear fundamental diagram. The estimation problem considers two key principles. First, the error minimization between the measured and reconstructed flows and densities, and second the equilibrium state of the network which establishes flow propagation within the network. Both principles are integrated together with the traffic model constraints established by the supply/demand paradigm. Finally the problem is cast as a constrained quadratic optimization with 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.

In [62], we addressed the conditions imposed on the number and location of fixed sensors such that all flows in the network can be uniquely reconstructed. We determine the minimum number of sensors needed to solve the problem given partial information of turning ratios, and then we propose a linear time algorithm for their allocation in a network. Using these results in addition to floating car data, we propose a method to reconstruct all traffic density and flow.

7.3.2. 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 [37], 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.

7.3.3. 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.

7.3.4. Dissipation of stop-and-go waves via control of autonomous vehicles

Participants: R. Stern, S. Cui, M. L. Delle Monache [Contact person], R. Bhadani, M. Bunting, M. Churchill, N. Hamilton, R. Haulcy, H. Pohlmann, F. Wu, B. Piccoli, B. Seibold, J. Sprinkle, D. B. Work.

Traffic waves are phenomena that emerge when the vehicular density exceeds a critical threshold. Considering the presence of increasingly automated vehicles in the traffic stream, a number of research activities have focused on the influence of automated vehicles on the bulk traffic flow. In [38], we demonstrate experimentally that intelligent control of an autonomous vehicle is able to dampen stop-and-go waves that can arise even in the absence of geometric or lane changing triggers. Precisely, our experiments on a circular track with more than 20 vehicles show that traffic waves emerge consistently, and that they can be dampened by controlling the velocity of a single vehicle in the flow. We compare metrics for velocity, braking events, and fuel economy across experiments. These experimental findings suggest a paradigm shift in traffic management: flow control will be possible via a few mobile actuators (less than 5%) long before a majority of vehicles have autonomous capabilities.

7.3.5. Cooperative adaptive cruise control over unreliable networks

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

Cooperative Adaptive Cruise Control (CACC) is a promising technique to increase highway throughput, safety and comfort for vehicles. Enabled by wireless communication, CACC allows a platoon of vehicles to achieve better performance than Adaptive Cruise Control; however, since wireless is employed, problems related to communication unreliability arise. In [45], we design a digital controller to achieve platoon stability, enhanced by an observer to increase robustness against packet losses. Our results confirms the interest of using an observer in combination with a local and cooperative digital controller.

7.3.6. Heterogeneity in synchronization: an adaptive control approach, with applications to vehicle platooning

Participants: S. Baldi, P. Frasca [Contact person].

Heterogeneity is a substantial obstacle to achieve synchronisation of interconnected systems (that is, in control) In order to overcome heterogeneity, advanced control techniques are needed, such as the use of "internal models" or of adaptive techniques. In a series of papers motivated by multi-vehicle platooning and coordinated autonomous driving, we have explored the application of adaptive control techniques. Our results cover both the cases of state-feedback [15] and of output-feedback [16], under the assumption that the topology of the interconnections has no circuits. Further investigation has shown that restrictive assumption can be relaxed (at least for state-feedback on some specific topologies) [47]. This understanding paves the road to use these techniques not only to stabilise heterogeneous platoons, but also to manage their merging or splitting operations [48].

7.3.7. Modeling traffic on roundabout

Participants: M. L. Delle Monache [Contact person], A. Rat, S. Hammond, B. Piccoli.

In [50] we introduce a Riemann solver for traffic flow on a roundabout with two lanes. The roundabout is modeled as a sequence of junctions. The Riemann solver provides a solution at junctions by taking into consideration traffic distribution, priorities, and the maximization of through flux. We prove existence and uniqueness of the solution of the Riemann problem and show some results numerically. This work stems from the fact that there is a general notion among transportation professionals that having a longer additional lane length at a double-lane roundabout entry yields better performances. In [55], we investigate this notion using Lighthill-Whitham-Richards Model. Using Lighthill- Whitham-Richards model, a double-lane roundabout with additional lane design at the entry is analyzed. The additional lane lengths are varied at the entry in order to study the effect of different additional lane lengths on roundabout performance. The results obtained with the PDE model were then compared with similar lane length variations in VISSIM.

7.3.8. Two dimensional models for traffic

Participants: S. Mollier, M. L. Delle Monache, C. Canudas de Wit [Contact person], B. Seibold.

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 starts with a simple model [33] for homogeneous network and where a preferred direction of traffic exists. Our aim is to extend gradually this model by adding complexity. As this approach is uncommon, we investigate a way to compare the results of this model with microsimulation in [73] using Aimsun. Then, in the literature, the network is mainly assumed to be homogeneous. However, in a large-scale scenario, it is unlikely that the traffic network characteristics–such as speed limit, number of lanes, or the network geometry–remain constant throughout the network. Therefore, we introduce a first extension [59] where the fundamental diagram is space-dependent and varies with respect to the area considered. Finally, we have studied more recently a possible way to relax the assumption of a preferred direction of flow by considering several layers of density such that each layer describe a different direction of flow. In this case, the model becomes a system of conservation and is hyperbolic-elliptic which imply special caution in the choice of the numerical method.

7.4. Multisensor data fusion for navigation

7.4.1. Sensors fusion for attitude estimation

Participants: H. Fourati [Contact person], Z. Zhou, J. Wu.

Attitude estimation consists in the determination of rigid body orientation in 3D space (principally in terms of Euler angles, rotation matrix, or quaternion). As a key problem for multisensor attitude determination, Wahba's problem has been studied for almost 50 years. In [42], we present 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-D equations based on quaternions. They are then investigated with pseudoinverse matrices establishing a linear solution to n-D 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 are derived, showing higher computation speed. 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. From other side, the integration of the Accelerometer and Magnetometer (AM) provides continuous, stable and accurate attitude information for land-vehicle navigation without magnetic distortion and external acceleration. However, magnetic disturbance and linear acceleration strongly degrade the overall system performance. As an important complement, the Global Navigation Satellite System (GNSS) produces the heading estimates, thus it can potentially benefit the AM system. Such a GNSS/AM system for attitude estimation is mathematically converted to a multi-observation vector pairs matching problem in [44]. The optimal and sub-optimal attitude determination and their time-varying recursive variants are all comprehensively investigated and discussed. The developed methods are named as the Optimal Linear Estimator of Quaternion (OLEQ), Suboptimal-OLEQ (SOLEQ) and Recursive-OLEQ (ROLEQ) for different application scenarios. The theory is established based on our previous contributions, and the multi-vector matrix multiplications are decomposed with the eigenvalue factorization. Some analytical results are proven and given, which provides the reader with a brand new viewpoint of the attitude determination and its evolution. With the derivations of the two-vector case, the n-vector case is then naturally formed. The algorithms are then implemented using the C++ programming language on the designed hardware with a GNSS module, three-axis accelerometer and three-axis magnetometer, giving an effective validation of them in real-world applications. In [39], a super fast attitude solution is obtained for consumer electronics accelerometer-magnetometer combination. The quaternion parameterizing the orientation is analytically derived from a least-square optimization that maintains very simple form. Like previously developed approaches, this algorithm does not require predetermined magnetometer reference vector. In [41], we present a novel sequential multiplicative quaternion attitude estimation method from various vector sensor outputs. The unique linear constitution of the algorithm leads to its specific name of Recursive Linear Quaternion Estimator (RLQE). The algorithm's architecture is designed to use each single pair of vector observation linearly so that the vector observations can be arbitrarily chosen and fused. The closed-form covariance of the RLQE is derived that builds up the existence of a highly reliable RLQE Kalman filter (RLQE-KF). In [65], to generate the virtual-gyro output in the case of gyroscope failures, virtual-gyro Kalman filter is established for angular rate estimation base on attitude estimation results.

7.4.2. Attitude estimation applied in augmented reality

Participants: H. Fourati [Contact person], T. Michel, P. Genevès, N. Layaïda.

We investigate the precision of attitude estimation algorithms in the particular context of pedestrian navigation with commodity smartphones and their inertial/magnetic sensors. A particular attention was paid to the study of attitude estimation in the context of augmented reality motions when using smartphones [32]. We report on an extensive comparison and experimental analysis of existing algorithms. We focus on typical motions of smartphones when carried by pedestrians. We use a precise ground truth obtained from a motion capture system. We test state-of-the-art and built-in attitude estimation techniques with several smartphones, in the presence of magnetic perturbations typically found in buildings. We discuss the obtained results, analyze advantages and limits of current technologies for attitude estimation in this context. Furthermore, we propose a new technique for limiting the impact of magnetic perturbations with any attitude estimation algorithm used in this context.

7.4.3. Attitude determination for satellite

Participants: H. Fourati [Contact person], S. Pourtakdoust, Csug Team, E. Kerstel.

Recently, we started to work on attitude estimation for satellites. In [29], we are focused on the development and verification of a heat attitude model (HAM) for satellite attitude determination. Within this context, the Sun and the Earth are considered as the main external sources of radiation that could affect the satellite surface temperature changes. Assuming that the satellite orbital position (navigational data) is known, the proposed HAM provides the satellite surface temperature with acceptable accuracy and also relates the net heat flux (NHF) of three orthogonal satellite surfaces to its attitude via the inertial to satellite transformation matrix. The proposed HAM simulation results are verified through comparison with commercial thermal analysis tools. The proposed HAM has been successfully utilized in some researches for attitude estimation, and further studies for practical implementations are still ongoing. Actually, we are establishing a project around quantum communication experiments under Nanobob CubeSat mission [28]. Some attitude estimation algorithms will be deployed to orient the satellite to the ground station.

7.4.4. Sensors fusion for distance measurement in pedestrian navigation

Participants: H. Fourati [Contact person], Z. Zhou, J. Wu.

We developed in [43] a foot-mounted pedestrian navigation system prototype with the emphasis on distance measuring with an inertial measurement unit (IMU) which implies the characteristics of pedestrian gait cycle and thus can be used as a crucial step indicator for distance calculation. An adaptive time- and frequency-domains joint distance measuring method is proposed by utilizing the means of behaviors classification. Two key issues are studied: step detection and step length determination. For the step detection part, first behavior classification along with state transition strategy is designed to identify typical pedestrian behaviors including standing still, walking, running and irregular swing. Then a four-stage step detection method is proposed to adaptively determine both step frequency and threshold in a flexible window. Based on the behavior classification results, a two-segment functional based step length model is established to adapt the walking and running behaviors.

NON-A POST Team

6. New Results

6.1. Implementation of finite- and fixed-time algorithms

In [22] several algorithms of implicit discretization for generalized homogeneous systems having discontinuity only at the origin are developed. They are based on the transformation of the original system to an equivalent one which admits an implicit or a semi-implicit discretization schemes preserving the stability properties of the continuous-time system. Namely, the discretized model remains finite-time stable (in the case of negative homogeneity degree), and practically fixed-time stable (in the case of positive homogeneity degree).

6.2. A solution to finite- and fixed-time estimation

The work [18] deals with the problem of finite-time and fixed-time observation of linear multiple input multiple output (MIMO) control systems. The proposed nonlinear dynamic observers guarantee convergence of the observer states to the original system state in a finite and in a fixed (defined *a priori*) time. Algorithms for the observers parameters tuning are also provided and a robustness analysis against input disturbances and measurement noises is carried out.

6.3. Numeric and analytic design of homogeneous Lyapunov functions

The problem of the synthesis of a homogeneous Lyapunov function for an asymptotically stable homogeneous system is studied in [10]. First, for systems with nonnegative degree of homogeneity, several expressions of homogeneous Lyapunov functions are derived, which depend explicitly on the supremum or the integral (over finite or infinite intervals of time) of the system solutions. Second, a numeric procedure is proposed, which ensures the construction of a homogeneous Lyapunov function.

6.4. Distributed finite-time estimation

In [29] the robust distributed estimation for a class of time-invariant plants is achieved via a finite-time observer, its error reaching zero after a finite time in the absence of perturbation. Two types of robustness are also shown. First, input-to-state stability with respect to measurement noises and additive perturbations is proven. Second, we demonstrate that the estimation error stays bounded in the presence of known transmission delays.

QUANTIC Project-Team

6. New Results

6.1. Simulation of quantum walks and fast mixing with classical processes

Participants: A. Sarlette

This is the final result of a line of work where we show that the mixing behavior of quantum walks on graphs can always be simulated by a classical "lifted Markov chain". This implies that quantum walks must satisfy a conductance bound on mixing speed, like classical Markov chains. Also current efficient quantum walk constructions are linked to classical processes that provide the same convergence speed. This excludes a simple characterization of quantum walk advantages in terms of bare mixing speed, as has been done by some previous authors comparing just to simple Markov chains. The question of efficient design of walks on graphs, on the basis of local graph queries and for specific applications, is thus brought back to the center of the focus for quantum walks. This collaborative work with F. Ticozzi (U. of Padova) has been published in [11].

As a follow-up on this work, we have developed algorithms in the latter sense: quantum walks on the basis of local design and which do speed up some applications. These last results have been presented as posters at conferences and will hopefully be part of next year's publications.

6.2. Adiabatic elimination for multi-partite open quantum systems with non-trivial zero-order dynamics

Participants: Paolo Forni, Alain Sarlette, Pierre Rouchon

We pursue the work initiated in our group during the thesis of Rémi Azouit, where we apply center manifold theory in order to reduce the model of a quantum system to its slowly contracting dynamics. Such model reduction is ubiquitous in models of coupled quantum systems where part of the system relaxes quickly towards an equilibrium situation, and acts as an environment for a system of interest. The extension presented in this work is the answer to a question by experimental physicists at Laboratoire Kastler Brossel (LKB), where they apply a strong drive which, in an 'intuitive model', would saturate so-called two-level-system impurities and thereby imply a particular behavior of frequency shift and dissipation on the target system (slow dynamics) as a function of drive characteristics. A good model for this situation involves, beyond a strongly dissipative environment, also a fast non-dissipative dynamics on the slowly contracting subsystem. Adding the latter into the model reduction was the purpose of this result. We analyze the experimental results and show that the model reduction allows us to explain the observed trends. This result led to a publication in collaboration with physicists Thibault Capelle, Emmanuel Flurin and Samule Deleglise from LKB [20].

Further extensions of adiabatic elimination formulas have been worked out during this year and will hopefully be part of next year's publications.

6.3. Exponential stochastic stabilization of a two-level quantum system via strict Lyapunov control

Participants: Gerardo Cardona, Alain Sarlette, Pierre Rouchon

In this result, we address the fundamental task of stabilizing the state of a quantum system towards a target eigenstate of a continuous-time quantum nondemolition measurement. The starting point is that a static output feedback does not allow us to stabilize this system, while more complicated procedures were not able to provide a convergence rate. Our main idea is to introduce a dynamic feedback controller of moderate complexity, where (i) feedback gains depend on estimated state and progressively go to zero as one approaches the target; and (ii) the feedback involves noise (in this paper from the measurement back-action but in further extensions possibly just independent noise). With this controller we show, providing a Lyapunov function close to the Bures distance measure, that the system converges exponentially towards the target eigenstate. This result, restricted to a proof-of-principle on the qubit, was published in [19].

This has laid the basis for further work, presented on posters and to be published next year, where we have shown that:

- the optimal convergence rate, equal to information gain, can be achieved with this feedback;

- the procedure extends to N-level systems, with noise just independent instead of coming from the measurement backaction;

- the procedure can be exploited towards continuous-time measurement-based quantum error correction

6.4. Structural instability of driven Josephson circuits prevented by an inductive shunt

Participants: Lucas Verney, Raphaël Lescanne, Zaki Leghtas, Mazyar Mirrahimi.

Superconducting circuits are a versatile platform to implement a multitude of Hamiltonians which perform quantum computation, simulation and sensing tasks. A key ingredient for realizing a desired Hamiltonian is the irradiation of the circuit by a strong drive. These strong drives provide an insitu control of couplings, which cannot be obtained by near-equilibrium Hamiltonians. However, as shown in our result, out-of-equilibrium systems are easily plagued by complex dynamics leading to instabilities. Predicting and preventing these instabilities is crucial, both from a fundamental and application perspective. We propose an inductively shunted transmon as the elementary circuit optimized for strong parametric drives. Developing a novel numerical approach that avoids the built-in limitations of perturbative analysis, we demonstrate that adding the inductive shunt significantly extends the range of pump powers over which the circuit behaves in a stable manner. This collaborative work between the Quantic team and Michel Devoret at Yale has been recently submitted for publication [25].

6.5. Observing the escape of a driven quantum Josephson circuit into unconfined states

Participants: Raphaël Lescanne, Lucas Verney, Mazyar Mirrahimi, Zaki Leghtas.

Josephson circuits have been ideal systems to study complex non-linear dynamics which can lead to chaotic behavior and instabilities. More recently, Josephson circuits in the quantum regime, particularly in the presence of microwave drives, have demonstrated their ability to emulate a variety of Hamiltonians that are useful for the processing of quantum information. In this experimental work, we show that these drives lead to an instability which results in the escape of the circuit mode into states that are not confined by the Josephson cosine potential. We observe this escape in a ubiquitous circuit: a transmon embedded in a 3D cavity. When the transmon occupies these free-particle-like states, the circuit behaves as though the junction had been removed, and all non-linearities are lost. This work deepens our understanding of strongly driven Josephson circuits, which is important for fundamental and application perspectives, such as the engineering of Hamiltonians by parametric pumping. This collaborative work between Quantic team, Benjamin Huard's team at ENS Lyon and Michel Devoret at Yale, has been recently submitted for publication [21].

6.6. Dynamics of a qubit while simultaneously monitoring its relaxation and dephasing

Participants: Zaki Leghtas.

Decoherence originates from the leakage of quantum information into external degrees of freedom. For a qubit, the two main decoherence channels are relaxation and dephasing. Here, we report an experiment on a superconducting qubit where we retrieve part of the lost information in both of these channels. We demonstrate that raw averaging of the corresponding measurement records provides a full quantum tomography of the qubit state where all three components of the effective spin-1/2 are simultaneously measured. From single realizations of the experiment, it is possible to infer the quantum trajectories followed by the qubit state conditioned on relaxation and/or dephasing channels. The incompatibility between these quantum measurements of the qubit leads to observable consequences in the statistics of quantum states. The high level of controllability of superconducting circuits enables us to explore many regimes from the Zeno effect to underdamped Rabi oscillations depending on the relative strengths of driving, dephasing, and relaxation. This work is a collaboration between the Quantic team and the group of Benjamin Huard at ENS Lyon and was published in [13].

6.7. Demonstration of an effective ultrastrong coupling between two oscillators

Participants: Zaki Leghtas

When the coupling rate between two quantum systems becomes as large as their characteristic frequencies, it induces dramatic effects on their dynamics and even on the nature of their ground state. The case of a qubit coupled to a harmonic oscillator in this ultrastrong coupling regime has been investigated theoretically and experimentally. Here, we explore the case of two harmonic oscillators in the ultrastrong coupling regime. Probing the properties of their ground state remains out of reach in natural implementations. Therefore, we have realized an analog quantum simulation of this coupled system by dual frequency pumping a nonlinear superconducting circuit. The pump amplitudes directly tune the effective coupling rate. We observe spectroscopic signature of a mode hybridization that is characteristic of the ultrastrong coupling. We experimentally demonstrate a key property of the ground state of this simulated ultrastrong coupling between modes by observing simultaneous single- and two-mode squeezing of the radiated field below vacuum fluctuations. This work is a collaboration between the Quantic team and the group of Benjamin Huard at ENS Lyon and was published in [14].

6.8. Fault-tolerant detection of a quantum error

Participants: Mazyar Mirrahimi

A critical component of any quantum error–correcting scheme is detection of errors by using an ancilla system. However, errors occurring in the ancilla can propagate onto the logical qubit, irreversibly corrupting the encoded information. We experimentally demonstrate a fault-tolerant error-detection scheme that suppresses spreading of ancilla errors by a factor of 5, while maintaining the assignment fidelity. The same method is used to prevent propagation of ancilla excitations, increasing the logical qubit dephasing time by an order of magnitude. Our approach is hardware-efficient, as it uses a single multilevel transmon ancilla and a cavity-encoded logical qubit, whose interaction is engineered in situ by using an off-resonant sideband drive. The results demonstrate that hardware-efficient approaches that exploit system-specific error models can yield advances toward fault-tolerant quantum computation. This work is a collaboration between the Quantic team and the group of Robert Schoelkopf at Yale university and was published in [17].

6.9. Coherent oscillations inside a quantum manifold stabilized by dissipation

Participants: Zaki Leghtas, Mazyar Mirrahimi

Manipulating the state of a logical quantum bit usually comes at the expense of exposing it to decoherence. Fault-tolerant quantum computing tackles this problem by manipulating quantum information within a stable manifold of a larger Hilbert space, whose symmetries restrict the number of independent errors. The remaining errors do not affect the quantum computation and are correctable after the fact. Here we implement the autonomous stabilization of an encoding manifold spanned by Schrödinger cat states in a superconducting cavity. We show Zeno-driven coherent oscillations between these states analogous to the Rabi rotation of a qubit protected against phase flips. Such gates are compatible with quantum error correction and hence are crucial for fault-tolerant logical qubits. This experimental work follows our previous theoretical proposal [70]. It is a collaboration between the Quantic team and the group of Michel Devoret at Yale university and was published in [18].

6.10. To catch and reverse a quantum jump mid-flight

Participants: Mazyar Mirrahimi

A quantum system driven by a weak deterministic force while under strong continuous energy measurement exhibits quantum jumps between its energy levels. This celebrated phenomenon is emblematic of the special nature of randomness in quantum physics. The times at which the jumps occur are reputed to be fundamentally unpredictable. However, certain classical phenomena, like tsunamis, while unpredictable in the long term, may possess a degree of predictability in the short term, and in some cases it may be possible to prevent a disaster by detecting an advance warning signal. Can there be, despite the indeterminism of quantum physics, a possibility to know if a quantum jump is about to occur or not? We answer this question affirmatively by experimentally demonstrating that the completed jump from the ground to an excited state of a superconducting artificial atom can be tracked, as it follows its predictable "flight," by monitoring the population of an auxiliary level coupled to the ground state. Furthermore, we show that the completed jump is continuous, deterministic, and coherent. Exploiting this coherence, we catch and reverse a quantum jump mid-flight, thus preventing its completion. This real-time intervention is based on a particular lull period in the population of the auxiliary level, which serves as our advance warning signal. Our experimental results, which agree with theoretical predictions essentially without adjustable parameters, support the modern quantum trajectory theory and provide new ground for the exploration of real-time intervention techniques in the control of quantum systems, such as early detection of error syndromes. This work is a collaboration between the Quantic team and the group of Michel Devoret at Yale university and is recently submitted for publication [22].

6.11. Remote entanglement stabilization and concentration by quantum reservoir engineering

Participants: Nicolas Didier, Jérémie Guillaud, Mazyar Mirrahimi

Quantum information processing in a modular architecture requires the distribution, stabilization, and distillation of entanglement in a qubit network. We present autonomous entanglement stabilization protocols between two superconducting qubits that are coupled to distant cavities. The coupling between cavities is mediated and controlled via a three-wave mixing device that generates either a two-mode squeezed state or a delocalized mode between the remote cavities depending on the pump applied to the mixer. Local drives on the qubits and the cavities steer and maintain the system to the desired qubit Bell state. Most spectacularly, even a weakly squeezed state can stabilize a maximally entangled Bell state of two distant qubits through an autonomous entanglement concentration process. Moreover, we show that such reservoir-engineering-based protocols can stabilize entanglement in the presence of qubit-cavity asymmetries and losses. This work was published in [12].

SPHINX Project-Team

6. New Results

6.1. Inverse problems for heterogeneous systems

Participants: David Dos Santos Ferreira, Karim Ramdani, Julie Valein, Alexandre Munnier, Jean-Claude Vivalda.

- In [32], we deal with a problem of observability for waves propagating in two environments with different speeds of propagation. We give an explicit construction of the regions of observability in the two-dimensional case. This allows us to determine in which locations we have to make some measurements in order to obtain the solution within the domain.
- In [33], we deal with the observability of the 1-D wave equation. The semi discretization of the waves problem leads to some uniform observability problems. This is due to the bad approximation of the high frequencies of discrete solutions. Some remedies are known, which involve finite element methods. In this paper, we give three methods allowing to retrieve the uniform observability when the approximations are made with a Galerkin method.
- In [15], Ramdani *et al.* proposed an algorithm for estimating from partial measurements the population for a linear age-structured population diffusion model. In this work, the physical parameters of the model were assumed to be known. The authors 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 [13], Munnier and Ramdani 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 [13], Munnier and Ramdani 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 [2], 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.
- In [18], we design a state observer for a coupled two dimensional partial differential equations (PDEs) system used to describe the heat transfer in a membrane distillation system for water desalination.

  In [23], we deal with uniqueness and stability issues for the inverse spectral problem of recovering the magnetic field and the electric potential in a Riemannian manifold from some asymptotic knowledge of the boundary spectral data of the corresponding Schrödinger operator under Dirichlet boundary conditions.

6.2. Control and stabilization of heterogeneous systems

Participants: Thomas Chambrion, David Dos Santos Ferreira, Takéo Takahashi, Julie Valein.

- 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 [27], we have proved a "Ball-Marsedn-Slemrod" obstruction to the bi-linear controllability of the Klein-Gordon equation. With different methods, we obtained comparable results for the Gross-Pitaevskii equation in [28].
- In [7], we study the local exponential stability of the nonlinear Korteweg-de Vries equation with boundary time-delay feedback by using two different methods: a Lyapunov functional approach (with an estimation on the decay rate, but with a restrictive assumption on the length of the spatial domain) and an observability inequality approach (for any non critical lengths).
- In [12], we study the local controllability to trajectories of a Burgers equation with nonlocal viscosity. By linearization we are led to an equation with a non local term whose controllability properties are analyzed by using Fourier decomposition and biorthogonal techniques. Once the existence of controls is proved and the dependence of their norms with respect to the time is established for the linearized model, a fixed point method allows us to deduce the result for the nonlinear initial problem.
- In [26], we establish a Lebeau-Robbiano spectral inequality for a degenerated one dimensional elliptic operator and show how it can be used to impulse control and finite time stabilization for a degenerated parabolic equation.
- In [25], We prove a Carleman estimate in a neighborhood of a multi-interface, under compatibility assumptions between the Carleman weight, the operators at the multi-interface, and the elliptic operators in the interior and the usual sub-ellipticity condition. We derive some properties of unique prolongation, control of the heat equation, and satblization of the related damped waves equation.

6.3. Numerical analysis and simulation of heterogeneous systems

Participant: Xavier Antoine.

- In [10], we design some accurate artificial boundary conditions for the semi-discretized linear Schrödinger and heat equations in rectangular domains. We show the accuracy of the method thanks to simulations
- In [5], we design fast numerical and highly accurate methods for the computation of steady states and the dynamics of time or space-fractional Schrödinger equations.
- In [1], we design a numerical model of diffusion for the study of the properties of noble gases originating from volcanic eruptions.
- In [4], the deal with a multilevel Schwarz Waveform Relaxation (SWR) Domain Decomposition Method (DDM) for the Non Linear Schrödinger Equation (NLSE).
- In [6], we design a fast and pseudo spectral preconditioned conjugated gradient method for the computation of the steady states related to the Gross-Pitaevskii equation with non local dipolar interaction.
- In [3], we deal with fractional microlocal analysis for the obtention of asymptotic estimates for the convergence of Schwarz Waveform Relaxation (SWR) domain decomposition method; this study is done is the two dimensional quantum case.
- In [11], we design new methods of very high order for the computation of diffracted fields; these methods rely on a B-splines finite element method and are related to the isogeometric analysis.
- In [17], we deal with the numerical analysis of fast and accurate schemes for solving one-dimensional time-fractional nonlinear Schrödinger equations set with artificial boundaries.

- In [35], we obtain a close approximation of the optimal parameters for the convergence of domain decomposition methods for the Schrödinger equation.
- In [19], we compute an explicit approximation of the optimal parameters for the convergence of domain decomposition methods for the Schrödinger equation.
- In [21], we introduce an original method in order to integrate PML in a pseudospectral method for the computation of the dynamics of the Dirac equation. Some applications to lasers are given.
- In [20], we deal with the asymptotic analysis of the rate of convergence of the classical and quasi-optimal Schwarz waveform relaxation (SWR) method for solving the linear Schrödinger equation.

6.4. Fluid-Structure Interaction

Participants: Julien Lequeurre, Jean-François Scheid.

In [16], we deal with shape optimization problem for a Stokes/elasticity system. The aim is to find the optimal shape of an elastic structure which minimizes an energy type functional. Results are obtained for a simplified free-boundary one-dimensional problem.

In [34], we design a hilbertian framework for the analysis of the planar Navier-Stokes (NS) equations either in vorticity or in stream function formulation. The fluid is assumed to occupy a bounded possibly multiply connected domain. The velocity field satisfies either homogeneous (no-slip boundary conditions) or prescribed Dirichlet boundary conditions. We prove that the proposed approach is equivalent to the classical one (stated in primitive variables, i.e. velocity and pressure fields) for strong and weak solutions. In particular . In particular, in both cases, we retrieve the pressure from the vorticity or the current function.

TRIPOP Team

6. New Results

6.1. Nonlinear waves in 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 oscillations (traveling breathers), or the scattering of vibrations through the chain. Such phenomena are strongly influenced by contact nonlinearities (Hertz force), spatial inhomogeneities and dissipation.

In the work [22], 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.

In reference [8], we analyze the discrete p-Schrödinger equation, an envelope equation that describes small oscillations in a Newton's cradle. In the limit when the exponent of the contact force lies slightly above unity, we derive three different continuum limits of the model which allow us to approximate the profiles of traveling breather solutions. One model consists of a logarithmic nonlinear Schrödinger equation which leads to a Gaussian approximation, and the two other are fully nonlinear degenerate Schrödinger equations which provide compacton approximations. These approximations are numerically validated by Newton-type computations. In the opposite (vibroimpact) limit when the exponent of the contact force is large, we obtain an analytical approximation of solitary waves in the form of a compacton.

6.2. Periodic motions of coupled impact oscillators

Participants: Guillaume James, Vincent Acary, Franck Pérignon.

In the work [17], 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.

6.3. 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 published in [11].
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.

6.4. Signal propagation along excitable chains

Participant: Arnaud Tonnelier.

Nonlinear self-sustained waves, or *autowaves*, have been identified in a large class of discrete excitable media. We have proposed a simple continuous-time threshold model for wave propagation in excitable media. The ability of the resulting transmission line to convey a one-bit signal is investigated. Existence and multistability of signals where two successive units share the same waveform is established. We show that, depending on the connectivity of the transmission line, an arbitrary number of distinct signals can be transmitted. More precisely, we prove that, for a one-dimensional information channel with nth-neighbor interactions, a n-fold degeneracy of the speed curve induces the coexistence of $2n$ propagating signals, n of which are stable and allow n distinct symbols transmission. The influence of model parameters (time constants, coupling strength and connectivity) on the traveling signal properties is analyzed. This work is almost finished and is going to be submitted.

6.5. 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 [1]. They form a particular class of dynamical systems whose simulation requires the development of specific methods for analysis and dedicated simulators [6].

6.5.1. 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 [3] [41] 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 [4].

6.5.2. Generalized-α scheme for nonsmooth multibody systems.

Participant: Vincent Acary.

This work [16] concerns a formalism for the transient simulation of nonsmooth dynamic mechanical systems composed of rigid and flexible bodies, kinematic joints and frictionless contact conditions. The proposed algorithm guarantees the exact satisfaction of the bilateral and unilateral constraints both at position and velocity levels. Thus, it significantly differs from penalty techniques since no penetration is allowed. The numerical scheme is obtained in two main steps. Firstly, a splitting method is used to isolate the contributions of impacts, which shall be integrated with only first-order accuracy, from smooth contributions which can be integrated using a higher order scheme. Secondly, following the idea of Gear, Gupta and Leimkuhler, the equation of motion is reformulated so that the bilateral and unilateral constraints appear both at position and velocity levels. After time discretization, the equation of motion involves two complementarity conditions and it can be solved at each time step using a monolithic semi-smooth Newton method. The numerical behaviour of the proposed method is studied and compared to other approaches for a number of numerical examples. Itis shown that the formulation offers a unified and valid approach for the description of contactconditions between rigid bodies as well as between flexible bodies.

6.5.3. Mechanics of musical instruments with contact and impacts.

Participants: Vincent Acary, Franck Pérignon.

Collisions in musical string instruments play a fundamental role in explaining the sound production in various instruments such as sitars, tanpuras and electric basses. Contacts occuring during the vibration provide a nonlinear effect which shapes a specific tone due to energy transfers and enriches the hearing experience. As such, they must be carefully simulated for the purpose of physically-based sound synthesis. Most of the numerical methods presented in the literature rely on a compliant modeling of the contact force between the string and the obstacle. In this contribution, numerical methods from nonsmooth contact dynamics are used to integrate the problem in time. A Moreau-Jean time-stepping scheme is combined with an exact scheme for phases with no contact, thus controlling the numerical dispersion. Results for a two-point bridge mimicking a tanpura and an electric bass are presented, showing the ability of the method to deal efficiently with such problems while invoking, as compared to a compliant approach, less modelling parameters and a reduced computational burden [7].

6.5.4. Numerical solvers for frictional contact problems.

Participants: Vincent Acary, Maurice Brémond.

In [15] report, we review several formulations of the discrete frictional contact problem that arises in space and time discretized mechanical systems with unilateral contact and three-dimensional Coulomb's friction. Most of these formulations are well–known concepts in the optimization community, or more generally, in the mathematical programming community. To cite a few, the discrete frictional contact problem can be formulated as variational inequalities, generalized or semi–smooth equations, second–order cone complementarity problems, or as optimization problems such as quadratic programming problems over second-order cones. Thanks to these multiple formulations, various numerical methods emerge naturally for solving the problem. We review the main numerical techniques that are well-known in the literature and we also propose new applications of methods such as the fixed point and extra-gradient methods with self-adaptive step rules for variational inequalities or the proximal point algorithm for generalized equations. All these numerical techniques are compared over a large set of test examples using performance profiles. One of the main conclusion is that there is no universal solver. Nevertheless, we are able to give some hints to choose a solver with respect to the main characteristics of the set of tests

6.5.4.1. Impact laws in chains of aligned balls

In [18] several "classical" multiple-impact laws are compared on chains of aligned balls: Moreau's law, the binary collision law, and the LZB approach [2]. Short analyses of these laws are made, and thorough comparisons are led numerically. It is concluded that both Moreau and the binary collision laws, furnish good results (in terms of predictability) only in very particular cases of elasticity coefficien, contact stiffenesses ratios, and mass ratios.

6.6. Analysis and Control of Set-Valued Systems

Participants: Bernard Brogliato, Christophe Prieur, Alexandre Vieira.

6.6.1. Higher-order sweeping process

This work [5] continues our previous results in [33], to the case when exogeneous terms are present in both the unilateral constraint, and in the dynamics. A suitable change of state variables allows one to recast the dynamics in a format that is close to the autonomous case, so that the well-posedness issues (existence and uniqueness of solutions) is shown (see the preprint [20] for a complete analysis, which in fact differs only slightly from the original one in [33]). The link with switching DAEs is made.

6.6.2. Robust sliding-mode control: continuous and discrete-time

This work [10] concerns the robust control of linear time-invariant systems, subjected to nonlinear varying state dependent disturbances as well as parameter uncertainties. A specific set-valued class of sliding-mode controllers is designed, and its discretization (with the implicit method introduced in [32], [34]) is analysed. One difficulty is that the parameter uncertainties, as well as the discretization, create unmatched disturbances. Stability and convergence results are proved. Let us mention also [9] that corrects a slight mistake in [80]. In the same way it is worth citing [14], [14] which continues the analysis of the implicit discretization of set-valued systems, this time oriented towards the consistency of time-discretizations for homogeneous systems, with one discontinuity at zero (sometimes called quasi-continuous, strangely enough).

6.6.3. Evolution variational inequalities

In [13] we continue our previous works on well-posedness and stabilization/control of a class of set-valued systems, that take the form of evolution variational inequalities. Dissipativity is then a key property. Regulation with state and output feedback, viability issues, are solved, with absolutely continuous and bounded variations solutions. Applications are in power converters.

6.6.4. Optimal control of LCS

The quadratic and minimum time optimal control of LCS as in (6) is tackled in [24], [25]. This work relies on the seminal results by Guo and ye (SIAM 2016), and aims at particularizing their results for LCS, so that they become numerically tractable and one can compute optimal controllers and optimal trajectories. The basic idea is to take advantage of the complementarity, to construct linear complementarity problems in the Pontryagin's necessary conditions which can then be integrated numerically, without having to guess a priori the switching instants (the optimal controller can eb discontinuous and the optimal trajectories can visit several modes of the complementarity conditions).

TROPICAL Project-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.

In a series of joint works with Antoine Hochart, we apply methods of non-linear fixed point theory to zero-sum games.

A key issue is the solvability of the ergodic equation associated to a zero-sum game with finite state space, i.e., given a dynamic programming operator T associated to an undiscounted problem, one looks for a vector u, called the bias, and for a scalar λ, the ergodic constant, such that $T(u) = \lambda e + u$. The bias vector is of interest as it allows to determine optimal stationnary strategies.

In [14], we studied zero-sum games with perfect information and finite action spaces, and showed that the set of payments for which the bias vector is not unique (up to an additive constant) coincides with the union of lower dimensional cells of a polyhedral complex, in particular, the bias vector is unique, generically. We provided an application to perturbation schemes in policy iteration.

In [36], we apply game theory methods to the study of the nonlinear eigenproblem for homogeneous order preserving self maps of the interior of the cone. We show that the existence and uniqueness of an eigenvector is governed by combinatorial conditions, involving dominions (sets of states "controlled" by one of the two players). In this way, we characterize the situation in which the existence of an eigenvector holds independently of perturbations, and we solve an open problem raised in [91].

In [15], we provide a representation theorem for "payment free" Shapley operators, showing that these are characterized by monotonicity and homogeneity axioms [15]. This extends to the two-player case known representation theorems for risk measures.

7.1.2. Nonlinear fixed point methods to compute joint spectral raddi of nonnegative matrices

Participants: Stéphane Gaubert, Nikolas Stott.

In [29], we introduce a non-linear fixed point method to approximate the joint spectral radius of a finite set of nonnegative matrices. We show in particular that the joint spectral radius is the limit of the eigenvalues of a family of non-linear risk-sensitive type dynamic programming operators. We develop a projective version of Krasnoselskii-Mann iteration to solve these eigenproblems, and report experimental results on large scale instances (several matrices in dimensions of order 1000 within a minute). The situation in which the matrices are not nonnegative is amenable to a similar approach [94].

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 [46], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [103], [109] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [82] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [32], [33], 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 with general volatilities. We study the convergence and obtain error estimates when the parameters and the value function are bounded. The more general quadratic growth case has been studied in the PhD manuscript [12].

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 [110], [111], the stochastic max-plus scheme proposed by Zheng Qu [118], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [116], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [61], the probabilistic numerical method of Fahim, Touzi and Warin [82]. We propose to associate and compare these methods in order to solve more general structures.

In a first work [35], we build a common framework for both the SDDP and a discrete time and finite horizon version of Zheng Qu's algorithm for deterministic problems involving a finite set-valued (or switching) control and a continuum-valued control. We propose an algorithm that generates monotone approximations of the value function as a pointwise supremum, or infimum, of basic (affine or quadratic for example) functions which are randomly selected. We give sufficient conditions that ensure almost sure convergence of the approximations to the value function.

7.1.5. Parametrized complexity of optimal control and zero-sum game problems

Participants: Marianne Akian, Stéphane Gaubert, Omar Saadi.

As already said above, the dynamic programing approach to optimal control and zero-sum game problems suffers of the curse of dimensionality. The aim of the PhD thesis is to unify different techniques to bypass this difficulty, in order to obtain new algorithms and new complexity results.

As a first step, we worked to extend an algorithm proposed by Sidford et al. in [126]. There, they proposed a randomized value iteration algorithm which improves the usual complexity bounds of the value iteration for *discounted* Markov Decision Problems (discrete time stochastic control problems). In a joint work with Zheng Qu (Hong Kong University), we are extending this algorithm to the ergodic (mean payoff) case, exploiting techniques from non-linear spectral theory [48]; this extension covers as well the case of two players (zero-sum).

7.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

7.2.1. Order isomorphisms and antimorphisms 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 [133] that if there exists an antimorphism on a finite-dimensional 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. This result was improved in [44], where we showed that the homogeneity assumption is not actually necessary: every antimorphism on a cone is automatically homogeneous of degree -1.

The study of the order isomorphisms of a cone goes back to Alexandrov and Zeeman, who considered maps preserving the light cone that arises in special relativity. This work was extended to more general cones by Rothaus; Noll and Schäffer; and Artstein-Avidan and Slomka. It was shown, in the finite-dimensional case, that all isomorphisms are linear if the cone has no one-dimensional factors. There are also some results in infinite dimension—however these are unsatisfactory because of the strong assumptions that must be made in order to get the finite-dimensional techniques to work. For example, a typical assumption is that the cone is the convex hull of its extreme rays, which is overly restrictive in infinite dimension. Using different techniques more suited to infinite dimension, we have been developing a necessary and sufficient criterion on the geometry of a cone for all its isomorphisms to be linear.

7.2.2. Horofunction compactifications of symmetric spaces

Participant: Cormac Walsh.

This work is in collaboration with Thomas Haettel (Montpellier), Anna-Sofie Schilling (Heidelberg), Anna Wienhard (Heidelberg).

The symmetric spaces form a fascinating class of geometrical space. These are the spaces in which there is a point reflection through every point. An example is the space $\mathrm{Pos}(\mathbb{C}, n)$ of positive definite $n \times n$ Hermitian matrices.

The interesting metrics on such spaces are the ones that are invariant under all the symmetries, in particular the invariant Finsler metrics. When the symmetric space is non-compact, as in the example just referred to, it is profitable to study the horofunction boundary of such metrics.

An important technique in trying to understand symmetric spaces is to look at their *flats*. These are subspaces that are, as their name suggests, flat in some sense. Because of the abundance of symmetries, there are many flats; indeed, every pair of points lies in a flat. Furthermore, given any two flats, there is a symmetry taking one to the other, and so they are all alike. It turns out that the restriction of an invariant Finsler metric to a single flat determines the metric everywhere, and gives the flat the geometry of a normed space.

Symmetric spaces can be compactified by means of the Satake compactification. In fact, there are several such compactifications, one associated to each irreducible faithful representation of the invariance group of the space. In [41], we show that each Satake compactification can be constructed as a horofunction compactification by choosing an appropriate invariant Finsler metric. In fact, the metrics we construct have polyhedral balls on the flat.

An important step in the proof is to show that the closure of a flat in the horofunction compactification of the symmetric space is the same as the horofunction compactification of the flat viewed as a metric space in its own right. This is not true for every metric space, since in general one might not be able to distinguish horofunctions by looking at a subspace.

7.2.3. The set of minimal upper bounds of two matrices in the Loewner order

Participant: Nikolas Stott.

A classical theorem of Kadison shows that the space of symmetric matrices equipped with the Loewner order is an anti-lattice, meaning that two matrices have a least upper bound if and only if they are comparable. In [24], we refined this theorem by characterizing the set of minimal upper bounds: we showed that it is homeomorphic to the quotient space $O(p) \setminus O(p,q)/O(q)$, where $O(p,q)$ denotes the orthogonal group associated to the quadratic form with signature (p,q), and $O(p)$ denotes the standard pth orthogonal group.

7.2.4. Generalization of the Hellinger distance

Participant: Stéphane Gaubert.

In [64] (joint work with Rajendra Bhatia of Ashoka University and Tanvi Jain, Indian Statistic Institute, New Delhi), we study some generalizations of the Hellinger distance to the space of positive definite matrices.

7.2.5. Spectral inequalities for nonnegative tensors and their tropical analogues

Participant: Stéphane Gaubert.

In [39] (joint work with Shmuel Friedland, University of Illinois at Chicago) we extend some characterizations and inequalities for the eigenvalues of nonnegative matrices, such as Donsker-Varadhan, Friedland-Karlin, Karlin-Ost inequalities, to nonnegative tensors. These inequalities are related to a correspondence between nonnegative tensors and ergodic control: the logarithm of the spectral radius of a tensor is given by the value of an ergodic problem in which instantaneous payments are given by a relative entropy. Some of these inequalities involve the tropical spectral radius, a limit of the spectral radius which we characterize combinatorially as the value of an ergodic Markov decision process.

7.3. Tropical algebra and convex geometry

7.3.1. Formalizing convex polyhedra in Coq

Participants: Xavier Allamigeon, Ricardo Katz [Conicet, Argentine].

In [20], 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 supporting tools provided by the Mathematical Components library and its tactic language. The benefit of 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.

7.3.2. Tropical totally positive matrices

Participant: Stéphane Gaubert.

In [22] (joint work with Adi Niv) we investigate the tropical analogues of totally positive and totally non-negative matrices, i.e, the images by the valuation of the corresponding classes of matrices over a non-archimedean field. We show in particular that tropical totally positive matrices essentially coincide with the Monge matrices (defined by the positivity of 2×2 tropical minors), arising in optimal transport, and compare the set of tropical totally positive matrices with the tropicalization of the totally positive Grassmannian.

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 [16], 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 $\operatorname{adj}(A) \det(A)^{-1}$, 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 [21] (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

Participant: Stéphane Gaubert.

We investigate in [40] (joint work with Marie McCaig) the volume of tropical polytopes, as well as the number of integer points contained in integer polytopes. We proved that even approximating these values for a tropical polytope given by its vertices is hard, with no approximation algorithm with factor $2^{\mathrm{poly}(m,n)}$ existing unless P = NP.

7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

7.4.1. 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 $\mathrm{LP}(A,b,c) \equiv \min\{c \cdot x \mid Ax \leq b,\ x \geq 0\}$ is defined as the set of the optimal solutions (x^μ, w^μ) of the barrier problems:

$$\begin{aligned} \text{minimize} \quad & c \cdot x - \mu(\sum_{j=1}^{n} \log x_j + \sum_{i=1}^{m} \log w_i) \\ \text{subject to} \quad & Ax + w = b,\ x > 0,\ w > 0 \end{aligned}$$

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 [128], 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 [77], [76], [79], [78]. In particular, by analogy with the classical Hirsch conjecture, Deza, Terlaky and Zinchencko [78] 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 [17], we prove that primal-dual log-barrier 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 piecewise-linear 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.

7.4.2. Tropicalization of semidefinite programming and its relation with stochastic games

Participants: Xavier Allamigeon, Stéphane Gaubert, Mateusz Skomra.

Semidefinite programming consists in optimizing a linear function over a spectrahedron. The latter is a subset of $\mathbb{R}^n$ defined by linear matrix inequalities, i.e., a set of the form

$$\left\{x \in \mathbb{R}^n : Q^{(0)} + x_1 Q^{(1)} + \cdots + x_n Q^{(n)} \succeq 0\right\}$$

where the $Q^{(k)}$ are symmetric matrices of order m, and $\succeq$ denotes the Loewner order on the space of symmetric matrices. By definition, $X \succeq Y$ if and only if $X - Y$ is positive semidefinite.

Semidefinite programming is a fundamental tool in convex optimization. It is used to solve various applications from engineering sciences, and also to obtain approximate solutions or bounds for hard problems arising in combinatorial optimization and semialgebraic optimization.

A general issue in computational optimization is to develop combinatorial algorithms for semidefinite programming. Indeed, semidefinite programs are usually solved via interior point methods. However, the latter provide an approximate solution in a polynomial number of iterations, provided that a strictly feasible initial solution. Semidefinite programming becomes a much harder matter if one requires an exact solution. The feasibility problem belongs to $\mathsf{NP}_{\mathbb{R}} \cap \mathsf{coNP}_{\mathbb{R}}$, where the subscript $\mathbb{R}$ refers to the BSS model of computation. It is not known to be in NP in the bit model.

We address semidefinite programming in the case where the field $\mathbb{R}$ is replaced by a nonarchimedean field, like the field of Puiseux series. In this case, methods from tropical geometry can be applied and are expected to allow one, in generic situations, to reduce semialgebraic problems to combinatorial problems, involving only the nonarchimedean valuations (leading exponents) of the coefficients of the input.

To this purpose, we first study tropical spectrahedra, which are defined as the images by the valuation of nonarchimedean spectrahedra. We establish that they are closed semilinear sets, and that, under a genericity condition, they are described by explicit inequalities expressing the nonnegativity of tropical minors of order 1 and 2. These results are presented in the preprint [60], with further results in the PhD thesis [13].

We show in [18] that the feasibility problem for a generic tropical spectrahedron is equivalent to solving a stochastic mean payoff game (with perfect information). The complexity of these games is a long-standing open problem. They are not known to be polynomial, however they belong to the class $\mathsf{NP} \cap \mathsf{coNP}$, and they can be solved efficiently in practice. This allows to apply stochastic game algorithms to solve nonarchimedean semidefinite feasibility problems. We obtain in this way both theoretical bounds and a practicable method which solves some large scale instances.

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, [124] disproved this conjecture. In [19], 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 and on our previous results [60] and [18].

In [27] and [13], we exploit the tropical geometry approach to introduce a condition number for stochastic mean payoff games (with perfect information). This condition number is defined as the maximal radius of a ball in Hilbert's projective metric, contained in a primal or dual feasible set. We show that the convergence time of value iteration is governed by this condition number, and derive fixed parameter tractability results.

7.4.3. *Tropical polynomial systems and colorful interior of convex bodies*

Participants: Marianne Akian, Marin Boyet, Xavier Allamigeon, Stéphane Gaubert.

The starting PhD thesis work of Marin Boyet, deals with the solution of tropical polynomial systems, with motivations from call center performance evaluation (see Section 7.6.1). We introduced a notion of colorful interior of a family of convex bodies, and showed that the solution of such a polynomial system reduces to linear programming if one knows a vector in the colorful interior of an associated family of Newton polytopes. Further properties of colorful interiors are currently investigated.

7.5. Tropical algebra, number theory and directed algebraic topology

7.5.1. *An arithmetic site of Connes-Consani type for number fields with narrow class number 1*

Participant: Aurélien Sagnier.

In 1995, A. Connes ([71]) gave a spectral interpretation of the zeroes of the Riemann zeta function involving the action of $\mathbb{R}_+^*$ on the sector $X = \mathbb{Q}_+^\times \backslash \mathbb{A}_\mathbb{Q}/\widehat{\mathbb{Z}}^\times$ of the adele class space $\mathbb{A}_\mathbb{Q}/\mathbb{Q}^*$ of the field of rational numbers. In [72], [74], the action of $\mathbb{R}_+^*$ on this sector X was shown to have a natural interpretation in algebraic geometry. This interpretation requires the use of topos theory as well as of the key ingredient of characteristic one namely the semifield $\mathbb{R}_{\max}$ familiar in tropical geometry. The automorphism group of this semifield is naturally isomorphic to $\mathbb{R}_+^*$ and plays the role of the Frobenius. As it turns out, its action on the points of a natural semiringed topos corresponds canonically to the above action on X. This semiringed topos is called the arithmetic site. In my PhD, I extended the construction of the arithmetic site, replacing the field of rational numbers by certain number fields. I considered the simplest complex case, namely that of imaginary quadratic fields on which we assume that the units are not reduced to ± 1 that is when K is either $\mathbb{Q}(\imath)$ or $\mathbb{Q}(\imath\sqrt{3})$. These results are presented in the submitted article [121]. In a further work, developed this year, I extended this construction, dealing now with number fields K with narrow class number 1. In fact, if we denote $\mathcal{U}_{\mathcal{O}_K}^+$ the totally positive units of $\mathcal{O}_K$, $\mathcal{O}_K^+$ the totally positive integers, $\widehat{\mathcal{O}_K^+}$ the topos of sets with a multiplicative action of totally positive integers of $\mathcal{O}_K^+$, $D_K = \mathrm{Conv}(\mathcal{U}_{\mathcal{O}_K}^+)$ and $\mathcal{C}_{\mathcal{O}_K} = \mathrm{Semiring}(\{\lambda D_K / \lambda \in \mathcal{O}_K^+\}) \cup \{\varnothing, \{0\}\}$, we consider the semiringed topos $(\widehat{\mathcal{O}_K^+}, (\mathcal{C}_{\mathcal{O}_K}, \mathrm{Conv}(\bullet \cup \bullet), +))$ and show for it similar properties as the one shown in my PhD thesis for the arithmetic sites associated to imaginary quadratic fields with class number 1 by adapting to this case the technics used in my PhD thesis, Shintani units theorem, and some remarks A.Connes made on my PhD which appear as an appendix of the article [121]. Here again tropical algebra play a crucial role in the geometrical constructions.

7.5.2. *Tropical tensor products*

Participants: Stéphane Gaubert, Aurélien Sagnier.

Tensors products of modules over semifields of characteristic one, like the Boolean or tropical semifields, have appeared recently, with motivations from arithmetics, in work by Connes and Consani, towards an intersection theory for arithmetic and scaling sites (spaces they have built and which are closely related to the zeroes of the Riemann zeta function). Algebraic and topological tropical tensors products were constructed in a different way by Litvinov and collaborators: here, tropical tensors are sums of "rank one" expressions, similar to the ones used in the approximation of large data sets or of functions of many parameters. We show that the canonical notion of tropical tensor product, defined in terms of the usual universal problem, differs from the definition arising from approximation theory, but that the latter can be recovered from the former by a certain "reduction" operation. We illustrate these results by computing several basic examples of categorical tensors products, including spaces of convex sets and functions.

7.5.3. Directed topological complexity and control

Participant: Aurélien Sagnier.

This is a joint work with Michael Farber and Eric Goubault.

The view we are taking here is that of topological complexity, as defined in [83], adapted to directed topological spaces.

Let us briefly motivate the interest of a directed topological complexity notion. It has been observed that the very important planification problem in robotics boils down to, mathematically speaking, finding a section to the path space fibration $\chi \ : \ PX = X^I \to X \times X$ with $\chi(p) = (p(0), p(1))$. If this section is continuous, then the complexity is the lowest possible (equal to one), otherwise, the minimal number of discontinuities that would encode such a section would be what is called the topological complexity of X. This topological complexity is both understandable algorithmically, and topologically, e.g. as s having a continuous section is equivalent to X being contractible. More generally speaking, the topological complexity is defined as the Schwartz genus of the path space fibration, i.e. is the minimal cardinal of partitions of $X \times X$ into “nice” subspaces F_i such that $s_{F_i} \ : \ F_i \to PX$ is continuous.

This definition perfectly fits the planification problem in robotics where there are no constraints on the actual control that can be applied to the physical apparatus that is supposed to be moved from point a to point b. In many applications, a physical apparatus may have dynamics that can be described as an ordinary differential equation in the state variables $x \in \mathbb{R}^n$ and in time t, parameterized by control parameters $u \in \mathbb{R}^p$, $\dot{x}(t) = f(t, x(t))$. These parameters are generally bounded within some set U, and, not knowing the precise control law (i.e. parameters u as a function of time t) to be applied, the way the controlled system can evolve is as one of the solutions of the differential inclusion $\dot{x}(t) \in F(t, x(t))$ where $F(t, x(t))$ is the set of all $f(t, x(t), u)$ with $u \in U$. Under some classical conditions, this differential inclusion can be proven to have solutions on at least a small interval of time, but we will not discuss this further here. Under the same conditions, the set of solutions of this differential inclusion naturally generates a dspace (a very general structure of directed space, where a preferred subset of paths is singled out, called directed paths, see e.g. [97]). Now, the planification problem in the presence of control constraints equates to finding sections to the analogues to the path space fibration (That would most probably not qualify for being called a fibration in the directed setting) taking a dipath to its end points. This notion is developed in this article, and we introduce a notion of directed homotopy equivalence that has precisely, and in a certain non technical sense, minimally, the right properties with respect to this directed version of topological complexity.

This notion of directed topological complexity also has applications in informatics where a directed space can be used to model the space of all possible executions of a concurrent process (ie when several running programs must share common limited ressources).

In a recent prepublication [84], after defining the notion of directed topological complexity,this invariant (directed topological complexity) is studied for directed spheres and directed graphs.

7.6. Applications

7.6.1. Performance evaluation of an emergency call center

Participants: Xavier Allamigeon, Stéphane Gaubert.

Since 2014, we have been collaborating with Préfecture de Police (Régis Reboul and LcL Stéphane Raclot), more specifically with Brigade de Sapeurs de Pompiers de Paris (BSPP) and Direction de Sécurité de Proximité de l'agglomération parisienne (DSPAP), on the performance evaluation of the new organization to handle emergency calls to firemen and policemen in the Paris area. We developed analytical models, based on Petri nets with priorities, and fluid limits, see [55], [56], [65]. In 2018, we performed specific case studies, with several students of École polytechnique: Laetitia de Coudenhove, Julie Poulet, Céline Moucer and Julia Escribe.

7.6.2. 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 deterministic analogue of first passage percolation. We showed that the fire tends to propagate according to a polyhedral shape, and derived metric limit theorems, exploiting discrete convexity results à la Shapley-Folkman. We validated this approach by simulations, on the fire following Kobe earthquake in 1995. The polyhedral shape is also apparent in historical fires, like the great fire of London (1666). These results are announced in [28].

7.6.3. Smart Data Pricing

Participants: Marianne Akian, Jean-Bernard Eytard, Stéphane Gaubert.

This work is in collaboration with Mustapha Bouhtou (Orange Labs) and with Gleb Koshevoy (Russian academy of Science).

The PhD work [81] 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 [80] and also in [34]. In a followup work, presented in [81], we managed to extend these results to wider classes of bilevel problems, and to relate them to competitive equilibria problems.

7.6.4. 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, Olivier Beaude and Cheng Wan (EDF Labs).

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 as it incitates 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 contributions are presented in [102], [23].

Another work, by Paulin Jacquot and Cheng Wan, deals with limit theorems for atomic games with a large number of players [30], [42].

BONUS Team

7. New Results

7.1. Decomposition-based optimization

- **A set-oriented decomposition algorithm for multi-objective optimization.**
  Participants: B. Derbel and A. Liefooghe, external collaborators: H. Aguirre and K. Tanaka, Shinshu University (JAPAN); S. Verel, Univ. Littoral (FRANCE); Q. Zhang, City University (HONG KONG)

  The working principles of the well-established multi-objective evolutionary algorithm MOEA/D relies on the iterative and cooperative improvement of a number of single-objective sub-problems obtained by decomposition. Besides the definition of sub-problems, selection and replacement are, like in any evolutionary algorithm, the two core elements of MOEA/D. We argue that these two components are however loosely coupled with the maintained population. Thereby, in [24], we propose to re-design the working principles of MOEA/D by adopting a set-oriented perspective, where a many-to-one mapping between sub-problems and solutions is considered. Selection is then performed by defining a neighborhood relation among solutions in the population set, depending on the corresponding sub-problem mapping. Replacement is performed following an elitist mechanism allowing the population to have a variable, but bounded, cardinality during the search process. By conducting a comprehensive empirical analysis on a range of combinatorial multi- and many-objective nk-landscapes, we show that the proposed approach leads to significant improvements, especially when dealing with an increasing number of objectives. Our findings indicate that a set-oriented design can constitute a sound alternative for strengthening the practice of multi- and many-objective evolutionary optimization based on decomposition.
- **Parallel Pareto local search for multi-objective optimization.**
  Participants: B. Derbel and A. Liefooghe, external collaborators: J. Shi and J. Sun, Xi'an Jiaotong University (CHINA); Q. Zhang, City University (HONG KONG)

  Pareto Local Search (PLS) is a simple, yet effective optimization approach dedicated to multi-objective combinatorial optimization. It can however suffer from a high computational cost, especially when the size of the Pareto optimal set is relatively large. Recently, incorporating decomposition in PLS had revealed a high potential, not only in providing high-quality approximation sets, but also in speeding-up the search process. In [30], using the bi-objective Unconstrained Binary Quadratic Programming (bUBQP) problem as an illustrative benchmark, we demonstrate some shortcomings in the resulting decomposition-guided Parallel Pareto Local Search (PPLS), and we propose to revisit the PPLS design accordingly. For instances with a priori unknown Pareto front shape, we show that a simple pre-processing technique to estimate the scale of the Pareto front can help PPLS to better balance the workload. Furthermore, we propose a simple technique to deal with the critically-important scalability issue raised by PPLS when deployed over a large number of computing nodes. Our investigations show that the revisited version of PPLS provides a consistent performance, suggesting that decomposition-guided PPLS can be further generalized in order to improve both parallel efficiency and approximation quality.
- **Archivers for the representation of the set of approximate solutions for MOPs.**
  Participants: E-G. Talbi, external collaborators: O. Schutze, C. Hernandez (Computer Science Department, Cinvestav, MEXICO), Q. Sun, Y. Naranjani (School of Engineering University of California, USA), R. Xiong (Department of Mechanics, University Tianjin, CHINA)

  In this work we have addressed the problem of computing suitable representations of the set of approximate solutions of a given multi-objective optimization problem via stochastic search algorithms. For this, we have proposed different archiving strategies for the selection of the candidate

solutions maintained by the generation process of the stochastic search process, and investigate them further on analytically and empirically. For all archivers we have provided upper bounds on the approximation quality as well as on the cardinality of the limit solution set. A comparative study on some test problems in order to visualize the effect of all novel archiving strategies has also been carried out [18].

7.2. ML-assisted optimization

FIve major contributions related to ML-assisted optimization have been achieved and summarized in the following. As pointed out previously in our research program, one of the major issues in surrogate-assisted optimization is how to integrate efficiently and effectively the surrogates in the optimization process. This issue is addressed in first three contributions. Another major aspect addressed in the fourth contribution is the investigation of surrogates within the context of combinatorial optimization. The focus of the fifth contribution is put on the landscape analysis applied within the context of multi-objective optimization.

- **Efficient Global Optimization Using Deep Gaussian Processes.**
  Participants: A. Hebbal, E-G. Talbi and N. Melab, external collaborators: L. Brevault and M. Balesdent from ONERA (Palaiseau, Paris)

  Efficient Global Optimization (EGO) is widely used for the optimization of computationally expensive black-box functions. EGO is based on a surrogate modeling technique using Gaussian Processes (kriging). However, due to the use of a stationary covariance, kriging is not well suited for approximating non stationary functions. Non stationarity is generally due to the abrupt change of a physical property that often occurs in the design of launch vehicles, subject of our collaboration with ONERA. This leads to a variation of the objective function with a completely different smoothness along the input space. In the spirit of deep learning using neural networks, we have investigated in [25] the integration of Deep Gaussian processes (DGP) in EGO framework to deal with non stationarity. Numerical experimentations are performed on analytical problems to highlight the different aspects of DGP and EGO. The experimental results show that the coupling EGO-DGP outperforms EGO-GP with a significant margin. Furthermore, the study has also highlighted some challenging issues to be investigated including: the integration of DGP in multi-objective EGO, the configuration of the network and revisiting the training model. Ultra-scale optimization at different levels is particularly important given the large number of hyperparameters of the training model.

- **Efficient global optimization of constrained mixed variable problems.**
  Participants: E-G. Talbi, external collaborators: Julien Pelamatti, Loïc Brevault, Mathieu Balesdent (ONERA) Yannick Guerin (CNES)

  Due to the increasing demand for high performance and cost reduction within the framework of complex system design, numerical optimization of computationally costly problems is an increasingly popular topic in most engineering fields [33]. In this work, several variants of the Efficient Global Optimization algorithm for costly constrained problems depending simultaneously on continuous decision variables as well as on quantitative and/or qualitative discrete design parameters are proposed. The adaptation that is considered is based on a redefinition of the Gaussian Process kernel as a product between the standard continuous kernel and a second kernel representing the covariance between the discrete variable values. Several parameterizations of this discrete kernel, with their respective strengths and weaknesses, have been investigated. The novel algorithms are tested on a number of analytical test-cases and an aerospace related design problem, and it is shown that they require fewer function evaluations in order to converge towards the neighborhoods of the problem optima when compared to more commonly used optimization algorithms [38].

- **Adaptive Evolution Control using Confident Regions for Surrogate-assisted Optimization.**
  Participants: G. Briffoteaux and N. Melab, external collaborators: M. Mezmaz and D. Tuyttens from Université de Mons (BELGIUM)

The challenge of the efficient/effective integration of surrogates in the optimization process is to find the best trade-off between the quality (in terms of quality/precision) of the generated solutions and the efficiency (in terms of execution time) of the resolution. In [22], we have investigated the evolution control that alternates between the real function (simulator) and the surrogate within the multi-objective optimization process. We propose an adaptive evolution control mechanism based on the distance-based concept of confident regions (hyperspheres). The approach has been integrated into an ANN-assisted NSGA-2 and experimented using the ZDT4 multi-modal benchmark function. The reported results show that the proposed approach outperforms two other existing ones.

- **A surrogate model for combinatorial optimization.**
  Participants: B. Derbel and A. Liefooghe, external collaborators: H. Aguirre and K. Tanaka, Shinshu University (JAPAN), S. Verel, Univ. Littoral (FRANCE)

  Extensive efforts so far have been devoted to the design of effective surrogate models for expensive black-box continuous optimization problems. There are, however, relatively few investigations on the development of methodologies for combinatorial domains. In [31], we rely on the mathematical foundations of discrete Walsh functions in order to derive a surrogate model for pseudo-boolean optimization functions. Specifically, we model such functions by means of Walsh expansion. By conducting a comprehensive set of experiments on nk-landscapes, we provide empirical evidence on the accuracy of the proposed model. In particular, we show that a Walsh-based surrogate model can outperform the recently-proposed discrete model based on Kriging.

- **Landscape analysis for multi-objective optimization.**
  Participants: B. Derbel and A. Liefooghe, external collaborators: H. Aguirre and K. Tanaka, Shinshu University (JAPAN); M. López-Ibánez, Univ. Manchester (UK); L. Paquete, Univ. Coimbra, Portugal; S. Verel, Univ. Littoral (FRANCE)

  Pareto local optimal solutions (PLOS) are believed to highly influence the dynamics and the performance of multi-objective optimization algorithms, especially those based on local search and Pareto dominance. In [28], we introduce a PLOS network (PLOS-net) model as a step toward the fundamental understanding of multi-objective landscapes and search algorithms. Using a comprehensive set of instances, PLOS-nets are constructed by full enumeration, and selected network features are further extracted and analyzed with respect to instance characteristics. A correlation and regression analysis is then conducted to capture the importance of the PLOS-net features on the runtime and effectiveness of two prototypical Pareto-based heuristics. In particular, we are able to provide empirical evidence for the relevance of the PLOS-net model to explain algorithm performance.

  Additionally, we know that local search algorithms naturally stop at a local optimal set (LO-set) under given definitions of neighborhood and preference relation among subsets of solutions, such as set-based dominance relation, hypervolume or epsilon indicator. It is an open question how LO-sets under different set preference relations relate to each other. In [29], we report an in-depth experimental analysis on multi-objective nk-landscapes. Our results reveal that, whatever the preference relation, the number of LO-sets typically increases with the problem non-linearity, and decreases with the number of objectives. We observe that strict LO-sets of bounded cardinality under set-dominance are LO-sets under both epsilon and hypervolume, and that LO-sets under hypervolume are LO-sets under set-dominance, whereas LO-sets under epsilon are not. Nonetheless, LO-sets under set-dominance are more similar to LO-sets under epsilon than under hypervolume. These findings have important implications for multi-objective local search. For instance, a dominance-based approach with bounded archive gets more easily trapped and might experience difficulty to identify an LO-set under epsilon or hypervolume. On the contrary, a hypervolume-based approach is expected to perform more steps before converging to better approximations.

7.3. Large scale GPU-centric optimization

Participants: J. Gmys, T. C. Pessoa and N. Melab, external collaborators: M. Mezmaz, D. Tuyttens from University of Mons (BELGIUM) and F.H. De Carvalho Junior from Universidade Federal Do Ceará (BRAZIL)

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 2018, in collaboration with A. Zomaya (The Univ. of Sydney) and I. Chakroun (IMEC, Leuven) N. Melab has (guest-)edited a special issue on this hot topic (editorial in [16]). In addition, we have put the focus on the investigation of these specific devices within the context of parallel optimization. In the following, two major contributions are reported: (1) Many-core Branch-and-Bound for GPU accelerators and MIC coprocessors; (2) Cuda Dynamic Parallelism (CDP) for backtracking.

- **Many-core Branch-and-Bound for GPU accelerators and MIC coprocessors.** Solving large optimization problems results in the generation of a very large pool of subproblems and the time-intensive evaluation of their associated lower bounds. Generating and evaluating those subproblems on coprocessors raises several issues including processor-coprocessor data transfer optimization, vectorization, thread divergence, etc. In [15], [32], we have investigated the offload-based parallel design and implementation of B&B algorithms for coprocessors addressing these issues. Two major many-core architectures are considered and compared: Nvidia GPU and Intel MIC. The proposed approaches have been experimented using the Flow-Shop scheduling problem and two hardware configurations equivalent in terms of energy consumption: Nvidia Tesla K40 and Intel Xeon Phi 5110P. The reported results show that the GPU-accelerated approach outperforms the MIC offload-based one even in its vectorized version. Moreover, vectorization improves the efficiency of the MIC offload-based approach with a factor of two.
- **Dynamic Configuration of CUDA Runtime Variables for CDP-based Divide-and-Conquer Algorithms.** CUDA Dynamic Parallelism (CDP) is an extension of the GPGPU programming model proposed to better address irregular applications and recursive patterns of computation. However, processing memory-demanding problems by using CDP is not straightforward, because of its particular memory organization. We have proposed in [23] (extension of [13]) an algorithm to deal with such an issue which dynamically calculates and configures the CDP runtime variables and the GPU heap on the basis of an analysis of the partial backtracking tree. We have implemented the algorithm for solving permutation problems and experimented on two test-cases: N-Queens and the Asymmetric Travelling Salesman Problem. The proposed algorithm allows different CDP-based backtracking from the literature to solve memory-demanding problems, adaptively with respect to the number of recursive kernel generations and the presence of dynamic allocations on GPU.

GEOSTAT Project-Team

7. New Results

7.1. Excitable systems

Participants: G. Attuel, E. Gerasimova-Chechkina, F. Argoul, H. Yahia, A. Arnéodo.

In a companion paper (I. Multifractal analysis of clinical data), we used a wavelet-based multiscale analysis to reveal and quantify the multifractal intermittent nature of the cardiac impulse energy in the low frequency range (2 Hz during atrial fibrillation (AF). It demarcated two distinct areas within the coronary sinus (CS) with regionally stable multifractal spectra likely corresponding to different anatomical substrates. The electrical activity also showed no sign of the kind of temporal correlations typical of cascading processes across scales, thereby indicating that the multifractal scaling is carried by variations in the large amplitude oscillations of the recorded bipolar electric potential. In the present study, to account for these observations, we explore the role of the kinetics of gap junction channels (GJCs), in dynamically creating a new kind of imbalance between depolarizing and repolarizing currents. We propose a one-dimensional (1D) spatial model of a denervated myocardium, where the coupling of cardiac cells fails to synchronize the network of cardiac cells because of abnormal transjunctional capacitive charging of GJCs. We show that this non-ohmic nonlinear conduction 1D modeling accounts quantitatively well for the "multifractal white noise" dynamics of the electrical activity experimentally recorded in the left atrial posterior wall area. We further demonstrate that the multifractal properties of the numerical impulse energy are robust to changes in the model parameters.

Publication: Frontiers in Physiology (in review forum).

7.2. Multiscale description in terms of multiplicative cascade, application to Earth observation signals

Participants: I. Hernandez-Carrasco, V. Garçon, J. Sudre, C. Garbe, H. Yahia.

A new methodology has been developed in order to improve the description of the spatial and temporal variability of not well-resolved oceanic variables from other well-observed high-resolution oceanic variables. The method is based on the cross-scale inference of information, incorporating the common features of different multifractal high-resolution variables into a coarser one. An exercise of validation of the methodology has been performed based on the outputs of coupled physical-biogeochemical Regional Ocean Modeling System adapted to the eastern boundary upwelling systems at two spatial resolutions. Once the algorithm has been proved to be effective in increasing the spatial resolution of modeled partial pressure of CO_2 at the surface ocean (pCO_2), we have investigated the capability of our methodology when it is applied to remote sensing data, focusing on the improvement of the temporal description. In this regard, we have inferred daily pCO_2 maps at high resolution (4 kms) fusing monthly pCO_2 data at low resolution (100 kms) with the small-scale features contained in daily high-resolution maps of satellite sea surface temperature and Chlorophyll-a. The algorithm has been applied to the South Eastern Atlantic Ocean opening the possibility to obtain an accurate quantification of the CO_2 fluxes in relevant coastal regions, such as the eastern boundary upwelling systems. Outputs of our algorithm have been compared with in situ measurements, showing that daily maps inferred from monthly products are in average 6 μatm closer to the in situ values than the original coarser monthly maps. Furthermore, values of pCO_2 have been improved in points close to the coast with respect to the original input data.

Publication: IEEE Transactions on Geoscience and Remote Sensing, HAL.

7.3. Multiscale description in terms of multiplicative cascade, application to Earth observation signals

Participants: H. Yahia, V. Garçon, J. Sudre, C. Maes.

We evidence and study the differences in turbulence statistics in ocean dynamics carried by wind forcing at the air-sea interface. Surface currents at the air-sea interaction are of crucial importance because they transport heat from low to high latitudes. At first order, oceanic currents are generated by the balance of the Coriolis and pressure gradient forces (geostrophic current) and the balance of the Coriolis and the frictional forces dominated by wind stress (Ekman current) in the surface ocean layers. The study was conducted by computing statistical moments on the shapes of spectra computed within the framework of microcanonical multi-fractal formalism. Remotely sensed daily datasets derived from one year of altimetry and wind data were used in this study, allowing for the computation of two kinds of vector fields: geostrophy with and geostrophy without wind stress forcing. We explore the statistical properties of singularity spectra computed from velocity norms and vorticity data, notably in relation with kurtosis information to underline the differences in the turbulent regimes associated with both kinds of velocity fields.

Publication: Frontiers of Information Technology & Electronic Engineering , Springer, 2018, 19 (8), HAL.

7.4. Multiscale description in terms of multiplicative cascade, application to Earth observation signals

Participants: A. El Aouni, K. Daoudi, H. Yahia, K. Minaoui.

We study coherent vortex detection from particles trajectories analysis and surface mixing and biological activity in the north african upwelling.

Publications: SIAM Conference on Nonlinear Waves and Coherent Structures HAL and AGU Ocean Sciences Meeting 2018 HAL.

7.5. Data-based identification of characteristic scales and automated modeling

Participants: N. Brodu, G. S. Phartiyal, D. Singh, H. Yahia.

Low-rankness transfer for denoising Sentinel-1 SAR images. Published in the 9th International Symposium on Signal, Image, Video and Communications ISIVC, Rabat, 2018, HAL.

A mixed spectral and spatial Convolutional Neural Network for Land Cover Classification using SAR and Optical data. Published in EGU General Assembly, Vienna, 2018, HAL.

Inferrence of causal states from time series for empirical modeling at prescribed scales. The goal of this research is to recover physical systems internal states from data and build a model of their evolution. Clustering together data with the same causal effets leads to consistent internal states: each measured data inferred to match the same state has by definition the same consequence, hence the same functional role. The theory behind this is well established, with major steps in the 80's by Jim Crutchfield. This leads to computational mechanics and epsilon-machines in the discrete case. The theory has however always suffers from computationability issues and it is very hard to apply in practice on large systems and real data. N. Brodu has made (unpublished) progress in 2018 in this theory, showing links between epsilon-machines and stochastic processes in the continuous case. The goal is to form a new class of algorithms drawing on the continuous representation, which would not suffer from the explicit discretization steps needed by current algorithms. N. Brodu has initiated a collaboration with Jim Crutchfield in 2017 and hope to further enhance that collaboration in 2019. This plan was presented to the reviewers during the team evaluation and deemed to be of high priority.

7.6. Speech analysis

Participants: G. Li, K. Daoudi, J. Klempir, J. Rusz, B. Das.

In the early stage of disease, the symptoms of Parkinson's disease (PD) are similar to atypical Parkinsonian sydromes (APS). The early differential diagnosis between PD and APS is thus a very challenging task. It trurns out that speech disorder is an early and common symptom to PD and APS. The goal of reserach is to develop a digital marker based on speech analysis in order to assist the neurologists in their diagnosis.

Publication: IEEE-ICASSP - 2018 IEEE International Conference on Acoustics, Speech and Signal Processing, Apr 2018, HAL.

7.7. InnovationLab with I2S, sparse signals & optimisation

Participants: M. Martin, A. Zebadua, S. Sakka, N. Brodu, K. Daoudi, A. Cherif [I2S], J. L. Vallancogne [I2S], A. Cailly [I2S].

During 2018 A. Zebadua was involved for the first time in the use of non-convex optimization methods and proximal operators, to solve inverse problems in image processing. Within the framework of the joint project with i2s, his main task was to work together with the research engineers to understand, implement, adapt and reduce the execution time of the algorithms developed by H. Badri in his doctoral thesis. These algorithms were developed in a scientific context, it was, therefore, necessary to adapt them to an industrial context with practical constraints.

S. Sakka has been implementating of the demosaicing algorithm to reconstruct a full-color image from raw images acquired by scanning. Colors are generated by a mask of Bayer. This algorithm uses the Hamilton Method and the Edge aware smoothing algorithm. He has been performing benchmarks for performance and quality test, and has written the technical report about the demosaicing algorithm. S. Sakka has been implementing iterative algorithms for linear system resolution useful for inpaitnig image processing algorithm.

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C. Sakka has been participating in the GPU Technology Conference organized by Nvidia in Munich and attending the NVIDIA Deep Learning School, and A. Zebadua has been participating to the winter school itwist18 in optimization from November 19th to 20th in Marseille.

M. Martin studied and made comparison between two methods : EAS (Edge Aware Smoothing) algorithm and LRT (low rank transfer) for denoising. She has been writing technical report to choose with I2S the best method : more efficient, less time. M. Martin has also been implementing denoising in C++ with librairy opencv and gpu. She has been setting up code sharing with I2S on gitlab Inria

INOCS Project-Team

7. New Results

7.1. Large scale complex structure optimization

Formulation and algorithms for last-mile delivery systems:

E-commerce is a thriving market around the world and suits very well the busy lifestyle of today's customers and this growing e-commerce poses a huge challenge for transportation companies, especially in the last mile delivery. We addressed first a fleet composition problem for last-mile delivery service. This problem occurs at a tactical level when the composition of the fleet has to be decided in advance. It is the case for companies that offer last-mile delivery service. Most of them subcontract the transportation part to local carriers and have to decide the day before which vehicles will be needed to cover a partially known demand. We assumed that the distribution area is divided into a limited number of delivery zones and the time horizon into time-slots. The demand is characterized by packages to be transported from pick-up zones to delivery zones given a delivery time slot. First, we introduced an integer programming model which aims to minimize the total delivery cost while ensuring that the demand is covered, the capacity of each vehicle is not violated, the working time for each period is not exceeded and the total working of each delivery respects the social regulations. Then we present a column-generation based approach, which is able to solve real-life instances in reasonable CPU times [33], [32]. Nowadays, the most common last mile delivery service is home delivery. Besides home delivery, companies like Amazon and Fedex, develop locker delivery. When customers shop online, they can choose a nearby locker as a pickup location. In the past years, a new concept called trunk delivery, has been proposed. Here, customers' orders can be delivered to the trunk of their cars. We jointly considered all these delivery possibilities in the same last-mile system and studied the case where the fleet is limited to a single vehicle. We proposed different formulations for the rising optimization problem. We developed problem defined cuts in order to strengthen the formulations and be able to tackle real-size instances. Last we designed and implemented a branch-and-cut algorithm [55], [53].

Large neighborhood algorithm for multi-commodity vehicle routing problem: When delivering fresh fruits and vegetables to catering the multi commodity aspect should be taken into account and deliveries to customers are not made in once, but each commodity can be delivered by a different vehicle as long as the total demand of that commodity is delivered. The problem that arises is the commodity constrained split delivery vehicle routing problem (C-SDVRP). We propose a heuristic based on the adaptive large neighborhood search (ALNS) to efficiently solve medium and large sized instances of the C-SDVRP. We take into account the distinctive features of the C-SDVRP and adapt several local search moves to improve a solution. Moreover, a mathematical programming based operator (MPO) that reassigns commodities to routes is used to improve a new global best solution. Computational experiments have been performed on benchmark instances from the literature. The results assess the efficiency of the algorithm, which can provide a large number of new best-known solutions in short computational times [50].

A matheuristic for the packaging and shipping problem: E-commerce has been continuously growing in the last years to a primary retail market. Recently in France, the threshold of 1 billion of online transactions was overcome. Due to a high demand fluctuation of e-commerce, the workforce sizing for the logistic chain is a challenging problem. Companies have to develop good strategies to have a sustainable workforce size while guaranteeing a high-level service. In this work, we consider the management of the workforce for a warehouse of an e-commerce company. Specifically, we address issues as i) How the workforce at the warehouse can be determined; ii) What is the daily operational production planning; iii) How the demand peaks can be smoothed, and the production maintained ideally constant over the time horizon. To provide answers to these issues, we introduce the Packaging and Shipping Problem (PSP). The PSP looks for a solution approach that jointly determines the workforce over a multi-period horizon and daily operational plans while minimizing the total logistics cost. We consider two strategies that aim to enhance the flexibility of the process and the efficiency

of resources use: reassignment and postponement. To tackle the Packaging and Shipping Problem we propose a model, and a three-phase matheuristic. This heuristic is proved to be competitive with respect to the direct solution of the model with a commercial solver on real-life based instances [18].

Heuristic and column generation approaches for the joint order batching and picker routing problem: Picking is the process of retrieving products from the inventory. It is mostly done manually by dedicated employees called pickers and is considered the most expensive of warehouse operations. To reduce the picking cost, customer orders can be grouped into batches that are then collected by traveling the shortest possible distance. We proposed an industrial case study for the HappyChic company where the warehouse has an acyclic layout: pickers are not allowed to backtrack. We developed a two-phase heuristic approach to solve this industrial case [59]. Moreover, we proposed an exponential linear programming formulation to tackle the joint order batching and picker routing problem. Variables, or columns, are related to the picking routes in the warehouse. Computing such routes is in general an intractable routing problem and relates to the well known traveling salesman problem (TSP). Nonetheless, the rectangular warehouse's layouts can be used to efficiently solve the corresponding TSP. Experimented on a publicly available benchmark, the algorithm proves to be very effective. It improves many of the best known solutions and provides very strong lower bounds. This approach is also applied to the HappyChic industrial case to demonstrate its interest for this field of application [41].

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 [21]. 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 H so as to maximize the minimum capacity margin over the feeders to avoid an overload for any feeder. A related theoretical work considers a very special case of hop constrained network design, namely the 2 edge-disjoint 3-paths polyhedron [15].

Switched Ethernet network design problems: We studied models arising in the design of switched Ethernet networks implementing the Multiple Spanning Tree Protocol [23]. 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.

Delay management in public transportation: The Delay Management Problem arises in Public Transportation networks, and is characterized by the necessity of connections between different vehicles. The attractiveness of Public Transportation networks is strongly related to the reliability of connections, which can be missed when delays or other unpredictable events occur. Given a single initial delay at one node of the network, the Delay Management Problem is to determine which vehicles have to wait for the delayed ones, with the aim of minimizing the dissatisfaction of the passengers. We derived strengthened mixed integer linear programming formulations and new families of valid inequalities for that problem. The implementation of branch-and-cut methods and tests on a benchmark of instances taken from real networks show the potential of the proposed formulations and cuts [20].

Discrete ordered median problem: The discrete ordered median problem consists in locating p facilities in order to minimize an ordered weighted sum of distances between clients and closest open facility. We formulate this problem as a set partitioning problem using an exponential number of variables. Each variable corresponds to a set of demand points allocated to the same facility with the information of the sorting position of their corresponding costs. We develop a column generation approach to solve the continuous relaxation of this model. Then, we apply a branch-price-and-cut algorithm to solve small to large sized instances of DOMP in competitive computational time [62].

Genome wide association studies: We studied the Polymorphic Alu Insertion Recognition Problem (PAIRP). Alu (Arthrobacter luteus) forms a major component of repetitive DNA and are frequently encountered during the genotyping of individuals. The basic approach to find Alus consists of (i) aligning sequence reads from a set of individual(s) with respect to a reference genome and (ii) comparing the possible Alu insertion induced by the alignment with the Alu insertions positions already known for the reference genome. The sequence genome of the reference individual is known and will be highly similar, but not identical, to the genome of the individual(s) being sequenced. Hence, at some locations they will diverge. Some of this divergence is due to the insertion of Alu polymorphisms. Detecting Alus has a central role in the field of Genetic Wide Association Studies because basic elements are a common source of mutation in humans. We investigated the PAIRP relationship with the the Clique Partitioning of Interval Graphs (CPIG). Our results [12], [26] provide insights of the complexity of the problem, a characterization of its combinatorial structure and an exact approach based on Integer Linear Programming to exactly solve the correspond instances.

A branch-and-cut algorithm for the maximum k-balanced subgraph of a signed graph: A signed graph is k-balanced if its vertex set can be partitioned into at most k sets in such a way that positive edges are found only within the sets and negative edges go between sets. The maximum k-balanced subgraph problem is the problem of finding a subgraph of G that is k-balanced and maximum according to the number of vertices. This problem has applications in clustering problems appearing in collaborative vs conflicting environments. We provide a representatives formulation for the problem and present a partial description of the associated polytope, including the introduction of strengthening families of valid inequalities. A branch-and-cut algorithm is described for finding an optimal solution to the problem. An ILS metaheuristic is implemented for providing primal bounds for this exact method and a branching rule strategy is proposed for the representatives formulation. Computational experiments, carried out over a set of random instances and on a set of instances from an application, show the effectiveness of the valid inequalities and strategies adopted in this work [22].

Feature selection in support vector machine: This work focuses on support vector machine (SVM) with feature selection. A MILP formulation is proposed for the problem. The choice of suitable features to construct the separating hyperplanes has been modelled in this formulation by including a budget constraint that sets in advance a limit on the number of features to be used in the classification process. We propose both an exact and a heuristic procedure to solve this formulation in an efficient way. Finally, the validation of the model is done by checking it with some well-known data sets and comparing it with classical classification methods [25].

7.2. Bilevel Programming

Pricing problems in energy management: Power systems face higher flexibility requirements from generation to consumption due to the increasing penetration of non-controllable distributed renewable energy. In this context, demand side management aims at reducing excessive load fluctuation and match the price of energy to their real cost for the grid. Pricing models for demand side management methods are traditionally used to control electricity demand. First, we proposed bilevel pricing models to explore the relationship between energy suppliers and customers who are connected to a smart grid. The smart grid technology allows customers to keep track of hourly prices and shift their demand accordingly, and allows the provider to observe the actual demand response to its pricing strategy. Moreover, we assumed that the smart grid optimizes the usage of a renewable energy generation source and a storage capacity. Results over a rolling horizon were obtained [14], [28], [36]. Next, we considered four types of actors: furnishers sell electricity, local agents trade and consume energy, aggregators trade energy and provide energy to end-users, who consume it. This gives rise to three levels of optimization. The interaction between aggregators and their end-users is modelled with a bilevel program, and so is the interaction between furnishers, and local agents and aggregators. Since solving bilevel programs is difficult in itself, solving trilevel programs requires particular care. We proposed three possible approaches, two of them relying on a characterization of the intermediary optimization level [35]. Finally, Time and-Level-of-Use is a recently proposed energy pricing scheme, designed for the residential

sector and providing suppliers with robust guarantee on the consumption. We formulate the supplier decision as a bilevel, bi-objective problem optimizing for both financial loss and guarantee. A decomposition method is proposed, related to the optimal value transformation. It allows for the computation of an exact solution by finding possible Pareto optimal candidate solutions and then eliminating dominated ones. Numerical results on experimental residential power consumption data show the method effectively finds the optimal candidate solutions while optimizing costs only or incorporating risk aversion at the lower-level [37].

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. In recent work, this approach was extended to include network capacities effects and a decoupling of prices in different zones [45], [46], [47], [48].

Market regulation: We proposed a bilevel programming model to study a problem of market regulation through government intervention. One of the main characteristics of the problem is that the government monopolizes the raw material in one industry, and competes in another industry with private firms for the production of commodities. Under this scheme, the government controls a state-owned firm to balance the market; that is, to minimize the difference between the produced and demanded commodities. On the other hand, a regulatory organism that coordinates private firms aims to maximize the total profit by deciding the amount of raw material bought from the state-owned firm. Two equivalent single-level reformulations are proposed to solve the problem. Additionally, three heuristic algorithms are designed to obtain good-quality solutions with low computational effort. Extensive computational experimentation is carried out to measure the efficiency of the proposed solution methodologies. A case study based on the Mexican petrochemical industry is presented. Additional instances generated from the case study are considered to validate the robustness of the proposed heuristic algorithms [66].

Rank pricing: One of the main concerns in management and economic planning is to sell the right product to the right customer for the right price. Companies in retail and manufacturing employ pricing strategies to maximize their revenues. The Rank Pricing Problem considers a unit-demand model with unlimited supply and uniform budgets in which customers have a rank-buying behavior. Under these assumptions, the problem is first analyzed from the perspective of bilevel pricing models and formulated as a non linear bilevel program with multiple independent followers. We also present a direct non linear single level formulation. Two different linearizations of the models are carried out and two families of valid inequalities are obtained which, embedded in the formulations by implementing a branch-and-cut algorithm, allow us to tighten the upper bound given by the linear relaxation of the models. We show the efficiency of the formulations, the branch-and-cut algorithms and some preprocessing through extensive computational experiments [16].

Bilevel minimum spanning tree problem: Consider a graph whose edge set is partitioned into a set of red edges and a set of blue edges, and assume that red edges are weighted and contain a spanning tree of G. Then, the Bilevel Minimum Spanning Tree Problem (BMSTP) consists in pricing (i.e., weighting) the blue edges in such a way that the total weight of the blue edges selected in a minimum spanning tree of the resulting graph is maximized. We propose different mathematical formulations for the BMSTP based on the properties of the Minimum Spanning Tree Problem and the bilevel optimization. We establish a theoretical and empirical comparison between these new formulations and we also provide reinforcements that together with a proper formulation are able to solve medium to big size instances [65].

Bilevel programming models for location problems: First, we addressed a multi-product location problem in which a retail firm has several malls with a known location. A particular product comes in p types. Each mall has a limited capacity for products to be sold at that location, so the firm has to choose what products to sold at what mall. Furthermore, the firm can apply discrete levels of discount on the products/ The objective of the firm is to find what products to sell at which mall, with what level of discount, so that its profit is maximized. Consumers are located in points of the region. Each consumer has a different set of acceptable products, and will purchase one of these, or none if it is not convenient for her. Consumers maximize their utility. The agents (firm and consumers) play a Stackelberg game, in which the firm is the leader and the customers the follower. Once the firm decides the products to sell at each mall and the possible discounts, consumers purchase (or not) one of their acceptable products wherever their utility is maximized. We model the problem using bilevel formulations, which are compared on known instances from the literature [43]. Second we studied a location problem of controversial facilities. On the one hand, a leader chooses among a number of fixed potential locations which ones to establish. On the second hand, one or several followers who, once the leader location facilities have been set, choose their location points in a continuous framework. The leader's goal is to maximize some proxy to the weighted distance to the follower's location points, while the follower(s) aim is to locate his location points as close as possible to the leader ones. We develop the bilevel location model for one follower and for any polyhedral distance, and we extend it for several followers and any so-called p-norm. We prove the NP-hardness of the problem and propose different mixed integer linear programming formulations. Moreover, we develop alternative Benders decomposition algorithms for the problem. Finally, we report some computational results comparing the formulations and the Benders decompositions on a set of instances [63].

Stackelberg games: First 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 [61].

Second, we formulate a Stackelberg Security game that coordinates resources in a border patrol problem. In this security domain, resources from different precincts have to be paired to conduct patrols in the border due to logistic constraints. Given this structure the set of pure defender strategies is of exponential size. We describe the set of mixed strategies using a polynomial number of variables but exponentially many constraints that come from the matching polytope. We then include this description in a mixed integer formulation to compute the Strong Stackelberg Equilibrium efficiently with a branch and cut scheme. Since the optimal patrol solution is a probability distribution over the set of exponential size, we also introduce an efficient sampling method that can be used to deploy the security resources every shift. Our computational results evaluate the efficiency of the branch and cut scheme developed and the accuracy of the sampling method. We show the applicability of the methodology by solving a real world border patrol problem [58].

7.3. Robust/Stochastic programming

Locating stations in a one-way electric car sharing system under demand uncertainty: We focused in [60] on a problem of locating recharging stations in one-way station based electric car sharing systems which operate under demand uncertainty. We modeled this problem as a mixed integer stochastic program and develop a Benders decomposition algorithm based on this formulation. We integrated a stabilization procedure to our algorithm and conduct a large-scale experimental study on our methods. To conduct the computational experiments, we developed a demand forecasting method allowing to generate many demand scenarios. The method was applied to real data from Manhattan taxi trips.

Integrated shift scheduling and load assignment optimization for attended home delivery: We studied an integrated shift scheduling and load assignment optimization problem for attended home delivery. The proposed approach is divided into two phases, each one corresponding to a different planning level: tactical and operational. In the tactical planning, a daily master plan is generated for each courier. This master plan defines the working shifts, the origin-destination pairs to visit, and the number of client requests to serve. In the operational planning, delivery orders are allocated to couriers in real-time. The stochastic and dynamic nature of client orders is included in the tactical and operational decision levels, respectively. For the tactical level, we developed and implemented a multi-cut L-shaped algorithm. Experimental results demonstrate that our approach provides robust tactical solutions that easily accommodate to fluctuations in client orders, preventing additional costs related to the underutilization of couriers and to the use of external couriers to satisfy all delivery requests, when compared to an approach using the mean demand value. Moreover, these results also indicate that the failure to incorporate robust tactical solutions in the operational planning results in infeasible operational plans that are inadmissible regarding the couriers' working time (e.g., minimum and maximum number of working hours) and work regulations (e.g., allocation of consecutive working hours to the couriers).

Bookings in the European gas market: Characterization of feasibility and computational complexity results: As a consequence of the liberalisation of the European gas market in the last decades, gas trading and transport have been decoupled. At the core of this decoupling are so-called bookings and nominations. Bookings are special long-term capacity right contracts that guarantee that a specified amount of gas can be supplied or withdrawn at certain entry or exit nodes of the network. These supplies and withdrawals are nominated at the day-ahead. These bookings then need to be feasible, i.e., every nomination that complies with the given bookings can be transported. While checking the feasibility of a nomination can typically be done by solving a mixed-integer nonlinear feasibility problem, the verification of feasibility of a set of bookings is much harder. We consider the question of how to verify the feasibility of given bookings for a number of special cases. For our physics model we impose a steady-state potential-based flow model and disregard controllable network elements. We derive a characterization of feasible bookings, which is then used to show that the problem is in coNP for the general case but can be solved in polynomial time for linear potential-based flow models. Moreover, we present a dynamic programming approach for deciding the feasibility of a booking in tree-shaped networks even for nonlinear flow models [56].

MISTIS Project-Team

7. New Results

7.1. Mixture models

7.1.1. Hierarchical 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. In the past year, we have been working on several extensions and applications of GLLiM as described below and the next two subsections.

We proposed a structured mixture model called Hierarchical Locally Linear Mapping (HGLLiM), to predict low-dimensional responses based on high dimensional covariates when the associations between the responses and the covariates are non-linear. For tractability, HGLLiM adopts inverse regression to handle the high dimension and locally-linear mappings to capture potentially non-linear relations. Data with similar associations are grouped together to form a cluster. A mixture is composed of several clusters following a hierarchical structure. This structure enables shared covariance matrices and latent factors across smaller clusters to limit the number of parameters to estimate. Moreover, HGLLiM adopts a robust estimation procedure for model stability. We used three real-world datasets to demonstrate different features of HGLLiM. With the face dataset, HGLLiM shows the ability of modeling non-linear relationship through mixtures. With the orange juice dataset, we show the prediction performance of HGLLiM is robust to the presence of outliers. Moreover, we demonstrated that HGLLiM is capable of handling large-scale complex data using the data acquired from a magnetic resonance vascular fingerprinting (MRvF) study. These examples illustrate the wide applicability of HGLLiM on handling different aspects of a complex data structure in prediction. A preliminary version of this work under revision for JRSS-C can be found in [72].

7.1.2. 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 [6] that bypasses the problems associated with high-to-low regression. The experimental validation of our method is performed in the context of vascular fingerprinting. The comparison between a standard grid search and the proposed approach suggest that MR Fingerprinting could benefit from a regression approach to limit dictionary size and fasten computation time. Preliminary tests and results have been presented at International Society for Magnetic Resonance in Medicine conference, ISMRM 2018 [35].

7.1.3. Massive analysis of multi-angular hyperspectral images of the planet Mars by inverse regression of physical models

Participants: Florence Forbes, Benoit Kugler.

Joint work with: Sylvain Douté from Institut de Planétologie et d'Astrophysique de Grenoble (IPAG).

In the starting PhD of Benoit Kugler, the objective is to develop a statistical learning technique capable of solving a complex inverse problem in planetary remote sensing. The challenges are 1) the large number of observations to to inverse, 2) their large dimension, 3) the need to provide predictions for correlated parameters and 4) the need to provide a quality index (eg. uncertainty). To achieve this goal, we have started to investigate a setting in which a physical model is available to provide simulations that can then be used for learning prior to inversion of real observed data. For the learning step to be as accurate as possible, an initial task is then to estimate the best fit of the theoretical model to the real data. We proposed an iterative procedure based on a combination of GLLiM [6] predictions and importance sampling steps.

7.1.4. Quantitative MRI Characterization of Brain Abnormalities in de novo Parkinsonian patients

Participants: Florence Forbes, Veronica Munoz Ramirez, Alexis Arnaud, Julyan Arbel.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience.

Currently there is an important delay between the onset of Parkinson's disease and its diagnosis. The detection of changes in physical properties of brain structures may help to detect the disease earlier. In this work, we proposed to take advantage of the informative features provided by quantitative MRI to construct statistical models representing healthy brain tissues. We used mixture models of non Gaussian distributions [8] to capture the non-standard shape of the data multivariate distribution. This allowed us to detect atypical values for these features in the brain of Parkinsonian patients following a procedure similar to that in [16]. Promising preliminary results demonstrate the potential of our approach in discriminating patients from controls and revealing the subcortical structures the most impacted by the disease. This work has been accepted at the IEEE International Symposium on Biological Imaging, ISBI 2019 [36].

7.1.5. No structural differences are revealed by voxel-based morphometry in de novo Parkinsonian patients

Participants: Florence Forbes, Veronica Munoz Ramirez.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience and Pierrick Coupé from Laboratoire Bordelais de Recherche en Informatique, UMR 5800, Univ. Bordeaux, Talence.

The identification of brain morphological alterations in newly diagnosed PD patients (i.e. de novo) could potentially serve as a biomarker and accelerate diagnosis. However, presently no consensus exists in the literature possibly due to several factors: small size cohorts, differences in segmentation techniques or bad control of false positive rates. In this study, we seek, using the Computational Anatomy Toolbox (CAT12) (University of Jena) pipeline, for morphological brain differences in gray and white matter of 66 controls and 144 de novo PD patients whose data were extracted from the PPMI (Parkinson Progressive Markers Initiative) database. Moreover, we searched for subcortical structure differences using the new online platform VolBrain (J. V. Manjón and P. Coupé, "volBrain: An Online MRI Brain Volumetry System," Front. Neuroinform., vol. 10, p. 30, Jul. 2016). We found no structural brain differences in this de novo Parkinsonian population, neither in tissues using a whole brain analysis nor in any of nine subcortical structures analyzed separately. We concluded that some results published in the literature appear as false positives and are not reproducible.

7.1.6. Characterization of daily glycemic variability in the patient with type 1 diabetes

Participants: Florence Forbes, Fei Zheng.

Joint work with: Stéphane Bonnet from CEA Leti and Pierre-Yves Benhamou, Manon Jalbert from CHU Grenoble Alpes.

Glycemic variability (GV) is an important component of glycemic control in patients with type 1 diabetes. Many metrics have been proposed to account for this variability but none is unanimous among physicians. One difficulty is that the variations in blood sugar levels are expressed very differently from one day to another in some subjects. Our goal was to develop and evaluate the performance of a daily GV index built by combining different known metrics (CV, MAGE, GVP etc). This in order to merge their descriptive power to obtain a more complete and more accurate index. This preliminary study will be presented at the Société Francophone du Diabète (SFD) in 2019 [46].

7.1.7. Glycemic variability improves after pancreatic islet transplantation in patients with type 1 diabetes

Participants: Florence Forbes, Fei Zheng.

Joint work with: Stéphane Bonnet from CEA Leti and Pierre-Yves Benhamou, Manon Jalbert from CHU Grenoble Alpes.

Glycemic variability (GV) must be taken into account in the efficacy of treatment of type 1 diabetes because it determines the quality of glycemic control, the risk of complication of the patient's disease. Our goal in this study was to describe GV scores in patients with pancreatic islet transplantation (PIT) type 1 diabetes in the TRIMECO trial, and change of thresholds, for each index. predictive of success of PIT.

7.1.8. Dirichlet process mixtures under affine transformations of the data

Participant: Julyan Arbel.

Joint work with: Riccardo Corradin from Milano Bicocca, Italy and Bernardo Nipoti from Trinity College Dublin, Ireland.

Location-scale Dirichlet process mixtures of Gaussians (DPM-G) have proved extremely useful in dealing with density estimation and clustering problems in a wide range of domains. Motivated by an astronomical application, in this work we address the robustness of DPM-G models to affine transformations of the data, a natural requirement for any sensible statistical method for density estimation. In [57], we first devise a coherent prior specification of the model which makes posterior inference invariant with respect to affine transformation of the data. Second, we formalize the notion of asymptotic robustness under data transformation and show that mild assumptions on the true data generating process are sufficient to ensure that DPM-G models feature such a property. As a by-product, we derive weaker assumptions than those provided in the literature for ensuring posterior consistency of Dirichlet process mixtures, which could reveal of independent interest. Our investigation is supported by an extensive simulation study and illustrated by the analysis of an astronomical dataset consisting of physical measurements of stars in the field of the globular cluster NGC 2419.

7.1.9. Applications of mixture models in Industry

Participant: Julyan Arbel.

Joint work with: Kerrie Mengersen, Earl Duncan, Clair Alston-Knox and Nicole White.

A very wide range of commonly encountered problems in industry are amenable to statistical mixture modelling and analysis. These include process monitoring or quality control, efficient resource allocation, risk assessment, prediction, and so on. Commonly articulated reasons for adopting a mixture approach include the ability to describe non-standard outcomes and processes, the potential to characterize each of a set of multiple outcomes or processes via the mixture components, the concomitant improvement in interpretability of the results, and the opportunity to make probabilistic inferences such as component membership and overall prediction.

In [51], We illustrate the wide diversity of applications of mixture models to problems in industry, and the potential advantages of these approaches, through a series of case studies.

7.1.10. Approximation results regarding the multiple-output mixture of the Gaussian-gated linear experts model

Participant: Florence Forbes.

Joint work with: Hien Nguyen, La Trobe University Melbourne Australia and Faicel Chamroukhi, Caen University, France.

Mixture of experts (MoE) models are a class of artificial neural networks that can be used for functional approximation and probabilistic modeling. An important class of MoE models is the class of mixture of linear experts (MoLE) models, where the expert functions map to real topological output spaces. Recently, Gaussian-gated MoLE models have become popular in applied research. There are a number of powerful approximation results regarding Gaussian-gated MoLE models, when the output space is univariate. These results guarantee the ability of Gaussian-gated MoLE mean functions to approximate arbitrary continuous functions, and Gaussian-gated MoLE models themselves to approximate arbitrary conditional probability density functions. We utilized and extended upon the univariate approximation results in order to prove a pair of useful results for situations where the output spaces are multivariate. We do this by proving a pair of lemmas regarding the combination of univariate MoLE models, which are interesting in their own rights.

7.1.11. Models for ranking data

Participant: Marta Crispino.

within the BigInsight project, Oslo.

We developed a new method and algorithms for working with ranking data. This kind of data is particularly relevant in applications involving personalized recommendations. In particular, we have invented a new Bayesian approach based on extensions of the Mallows model, which allows making personalized recommendations equipped with a level of uncertainty.

The Mallows model (MM) is a popular parametric family of models for ranking data, based on the assumption that a modal ranking, which can be interpreted as the consensus ranking of the population, exists. The probability of observing a given ranking is then assumed to decay exponentially fast as its distance from the consensus grows. The MM is therefore a two-parameter distance-based family of models. The scale or precision parameter, controlling the concentration of the distribution determines the rate of decay of the probability of individual ranks. Individual models with different properties can be obtained depending on the choice of distance on the space of permutations. A major drawback of the MM is that its computational complexity has limited its use to a particular form based on Kendall distance. We develop new computationally tractable methods for Bayesian inference in Mallows models that work with any right-invariant distance. Our method performs inference on the consensus ranking of the items, also when based on partial rankings, such as top-k items or pairwise comparisons. When assessors are many or heterogeneous, we propose a mixture model for clustering them in homogeneous subgroups, with cluster specific consensus rankings. We develop approximate stochastic algorithms that allow a fully probabilistic analysis, leading to coherent quantifications of uncertainties, make probabilistic predictions on the class membership of assessors based on their ranking of just some items, and predict missing individual preferences, as needed in recommendation systems. The methodology has been published in the Journal of Machine Learning Research, JMLR, in early 2018.

A generalization of the model above involves dealing with non-transitive and heterogeneous pairwise comparison data, coming from an experiment within the musicology domain. We thus develop a mixture model extension of the Bayesian Mallows model able to handle non-transitive data, with a latent layer of uncertainty which captures the generation of preference misreporting. This paper was recently accepted for publication in the Annals of Applied Statistics, AoAS.

Within this project, we also write a survey paper, whose main goal is to compare the performance of our method with other existing methodologies, including the Plackett-Luce, the Bradley-Terry, the collaborative filtering methods, and some of their variations. We illustrate and discuss the use of these models by means of an experiment in which assessors rank potatoes, and with a simulation. The purpose of this paper is not to recommend the use of one best method, but to present a palette of different possibilities for different questions and different types of data. This was recently accepted on the Annual Review of Statistics and Its Applications, ARSIA.

7.2. Semi and non-parametric methods

7.2.1. 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 α-quantile of the loss distribution. The Value-at-Risk however suffers from several weaknesses. First, it provides us only with a pointwise information: VaR(α) does not take into consideration what the loss will be beyond this quantile. Second, random loss variables with light-tailed distributions or heavy-tailed distributions may have the same Value-at-Risk. Finally, Value-at-Risk is not a coherent risk measure since it is not subadditive in general. A first coherent alternative risk measure is the Conditional Tail Expectation (CTE), also known as Tail-Value-at-Risk, Tail Conditional Expectation or Expected Shortfall in case of a continuous loss distribution. The CTE is defined as the expected loss given that the loss lies above the upper α-quantile of the loss distribution. This risk measure thus takes into account the whole information contained in the upper tail of the distribution. In [20], 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. However, the asymptotic normality of the empirical CTE estimator requires that the underlying distribution possess a finite variance; this can be a strong restriction in heavy-tailed models which constitute the favoured class of models in actuarial and financial applications. One possible solution in very heavy-tailed models where this assumption fails could be to use the more robust Median Shortfall, but this quantity is actually just a quantile, which therefore only gives information about the frequency of a tail event and not about its typical magnitude. In [65], we construct a synthetic class of tail L_p -medians, which encompasses the Median Shortfall (for $p = 1$) and Conditional Tail Expectation (for $p = 2$). We show that, for $1 < p < 2$, a tail L_p -median always takes into account both the frequency and magnitude of tail events, and its empirical estimator is, within the range of the data, asymptotically normal under a condition weaker than a finite variance. We extrapolate this estimator, along with another technique, to proper extreme levels using the heavy-tailed framework. The estimators are showcased on a simulation study and on a set of real fire insurance data showing evidence of a very heavy right tail.

A possible coherent alternative risk measure is based on expectiles [18], [63], [62]. 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.

7.2.2. Extrapolation limits associated with extreme-value methods

Participants: Clément Albert, Stéphane Girard.

Joint work with: L. Gardes (Univ. Strasbourg) and A. Dutfoy (EDF R&D).

The PhD thesis of Clément Albert (co-funded by EDF) is dedicated to the study of the sensitivity of extreme-value methods to small changes in the data and to their extrapolation ability. Two directions are explored:

(i) In [54], we investigate the asymptotic behavior of the (relative) extrapolation error associated with some estimators of extreme quantiles based on extreme-value theory. It is shown that the extrapolation error can be interpreted as the remainder of a first order Taylor expansion. Necessary and sufficient conditions are then provided such that this error tends to zero as the sample size increases. Interestingly, in case of the so-called Exponential Tail estimator, these conditions lead to a subdivision of Gumbel maximum domain of attraction into three subsets. In constrast, the extrapolation error associated with Weissman estimator has a common behavior over the whole Fréchet maximum domain of attraction. First order equivalents of the extrapolation error are then derived and their accuracy is illustrated numerically.

(ii) In [53], We propose a new estimator for extreme quantiles under the log-generalized Weibull-tail model, introduced by Cees de Valk. This model relies on a new regular variation condition which, in some situations, permits to extrapolate further into the tails than the classical assumption in extreme-value theory. The asymptotic normality of the estimator is established and its finite sample properties are illustrated both on simulated and real datasets.

7.2.3. Estimation of local intrinsic dimensionality with extreme-value methods

Participant: Stéphane Girard.

Joint work with: L. Amsaleg (LinkMedia, Inria Rennes), O. Chelly (NII Japon), T. Furon (LinkMedia, Inria Rennes), M. Houle (NII Japon), K.-I. Kawarabayashi (NII Japon), M. Nett (Google).

This work is concerned with the estimation of a local measure of intrinsic dimensionality (ID). The local model can be regarded as an extension of Karger and Ruhl's expansion dimension to a statistical setting in which the distribution of distances to a query point is modeled in terms of a continuous random variable. This form of intrinsic dimensionality can be particularly useful in search, classification, outlier detection, and other contexts in machine learning, databases, and data mining, as it has been shown to be equivalent to a measure of the discriminative power of similarity functions. In [14], several estimators of local ID are proposed and analyzed based on extreme value theory, using maximum likelihood estimation, the method of moments, probability weighted moments, and regularly varying functions. An experimental evaluation is also provided, using both real and artificial data.

7.2.4. Bayesian inference for copulas

Participants: Julyan Arbel, Marta Crispino, Stéphane Girard.

We study in [58] a broad class of asymmetric copulas known as Liebscher copulas and defined as a combination of multiple—usually symmetric—copulas. The main thrust of this work is to provide new theoretical properties including exact tail dependence expressions and stability properties. A subclass of Liebscher copulas obtained by combining Fréchet copulas is studied in more details. We establish further dependence properties for copulas of this class and show that they are characterized by an arbitrary number of singular components. Furthermore, we introduce a novel iterative construction for general Liebscher copulas which *de facto* insures uniform margins, thus relaxing a constraint of Liebscher's original construction. Besides, we show that this iterative construction proves useful for inference by developing an Approximate Bayesian computation sampling scheme. This inferential procedure is demonstrated on simulated data.

In [22], we investigate the properties of a new transformation of copulas based on the co-copula and an univariate function. It is shown that several families in the copula literature can be interpreted as particular outputs of this transformation. Symmetry, association, ordering and dependence properties of the resulting copula are established.

7.2.5. Bayesian nonparametric clustering

Participant: Julyan Arbel.

Joint work with: Riccardo Corradin from Milano Bicocca, Michal Lewandowski from Bocconi University, Milan, Italy, Caroline Lawless from Université Paris-Dauphine, France.

For a long time, the Dirichlet process has been the gold standard discrete random measure in Bayesian nonparametrics. The Pitman–Yor process provides a simple and mathematically tractable generalization, allowing for a very flexible control of the clustering behaviour. Two commonly used representations of the Pitman–Yor process are the stick-breaking process and the Chinese restaurant process. The former is a constructive representation of the process which turns out very handy for practical implementation, while the latter describes the partition distribution induced. Obtaining one from the other is usually done indirectly with use of measure theory. In contrast, we propose in [66] an elementary proof of Pitman–Yor's Chinese Restaurant process from its stick-breaking representation.

In the discussion paper [56], we propose a simulation study to emphasise the difference between Variation of Information and Binder's loss functions in terms of number of clusters estimated by means of the use of the Markov chain Monte Carlo output only and a "greedy" method.

The chapter [47] is part of a book edited by Stéphane Girard and Julyan Arbel. It presents a Bayesian nonparametric approach to clustering, which is particularly relevant when the number of components in the clustering is unknown. The approach is illustrated with the Milky Way's globulars, that are clouds of stars orbiting in our galaxy. Clustering globulars is key for better understanding the Milky Way's history. We define the Dirichlet process and illustrate some alternative definitions such as the Chinese restaurant process, the Pólya Urn, the Ewens sampling formula, the stick-breaking representation through some simple *R* code. The Dirichlet process mixture model is presented, as well as the *R* package *BNPmix* implementing Markov chain Monte Carlo sampling. Inference for the clustering is done with the variation of information loss function.

7.2.6. 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.

7.2.7. Extraction and data analysis toward "industry of the future"

Participants: Florence Forbes, Hongliang Lu, Fatima Fofana, 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.

7.2.8. Change point detection for the analysis of dynamic single molecules

Participants: Florence Forbes, Theo Moins.

Joint work with: Virginie Stoppin-Mellet from Grenoble Institute of Neuroscience.

The objective of this study was to develop a statistical learning technique to analyze signals produced by molecules. The main difficulties are the noisy nature of the signals and the definition of a quality index to allow the elimination of poor-quality data and false positive signals. In collaboration with the GIN, we addressed the statistical analysis of intensity traces (2 month internship of Theo Moins, Ensimag 2A). Namely, the ImageJ Thunderstorm toolbox, which has been developed for the detection of single molecule in super resolution imaging, has been successfully used to detect immobile single molecules and generate time-dependent intensity traces. Then the R package Segmentor3IsBack, a fast segmentation algorithm based on 5 possible statistical models, proved efficient in the processing of the noisy intensity traces. This preliminary study led to a multidisciplinary project funded by the Grenoble data institute for 2 years in which we will also address additional challenges for the tracking of a large population of single molecules.

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. A first version of this work can be found in [71] and has been presented at the JFRB 2018 workshop [41].

7.3.2. Robust structure learning using multivariate t-distributions

Participants: Karina Ashurbekova, Florence Forbes.

Joint work with: Sophie Achard, senior researcher at CNRS, Gipsa-lab.

Structure learning is an active topic nowadays in different application areas, i.e. genetics, neuroscience. We addressed the issue of robust graph structure learning in continuous settings. We focused on sparse precision matrix estimation for its tractability and ability to reveal some measure of dependence between variables. For this purpose, we proposed to extract good features from existing methods, namely *tlasso* and CLIME procedures. The former is based on the observation that standard Gaussian modelling results in procedures that are too sensitive to outliers and proposes the use of t-distributions as an alternative. The latter is an alternative to the popular Lasso optimization principle which can handle some of its limitations. We then combined these ideas into a new procedure referred to as tCLIME that can be seen as a modified *tlasso* algorithm. Numerical performance was investigated using simulated data and reveals that tCLIME performs favorably compared to the other standard methods. This work was presented at the Journées de Statistiques de la Société Francaise de Statistique in Saclay, 2018, [39].

7.3.3. Structure learning via Hadamard product of correlation and partial correlation matrices

Participants: Karina Ashurbekova, Florence Forbes.

Joint work with: Sophie Achard, senior researcher at CNRS, Gipsa-lab.

Classical conditional independences or marginal independences may not be sufficient to express complex relationships. In this work we introduced a new structure learning procedure where an edge in the graph corresponds to a non zero of both correlation and partial correlation. A theoretical study was derived which shows the good properties of the proposed graph estimator, illustrated also on a synthetic example.

7.3.4. 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 [16], 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.

7.3.5. 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. The results prove that the simultaneous inversion of both problems is well performed for simulation 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 have been presented at the SPIE medical imaging 2018 conference in Houston, USA [37].

7.3.6. 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. This work has been presented at the Joint Statistical Meeting in Vancouver Canada [29] and at the Journées de la Statistique in Saclay [40].

7.3.7. 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 [80]. 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 developed integrated models coupling EEG and eye movements within one single HMM for better identification of the phases. Here, the coupling incorporates 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 had to be added into the model, for the sake of synchronizing both processes. An associated EM algorithm for maximum likelihood parameter estimation was derived.

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 implement and validate our coupled model for jointly analyzing eye-movements and EEGs in order to improve the discrimination of the reading strategies.

7.3.8. Lossy compression of tree structures

Participant: Jean-Baptiste Durand.

Joint work with: Christophe Godin and Romain Azaïs (Inria Mosaic)

The class of self-nested trees presents remarkable compression properties because of the systematic repetition of subtrees in their structure. The aim of our work is to achieve compression of any unordered tree by finding the nearest self-nested tree. Solving this optmization problem without more assumptions is conjectured to be an NP-complete or NP-hard problem. In [34], we firstly provided a better combinatorial characterization of this specific family of trees. In particular, we showed from both theoretical and practical viewpoints that complex queries can be quickly answered in self-nested trees compared to general trees. We also presented an approximation algorithm of a tree by a self-nested one that can be used in fast prediction of edit distance between two trees.

Our goal for this coming year is to apply this approach to quantify the degree of self-nestedness of several plant species and extend first results obtained on rice panicles stating that near self-nestedness is a fairly general pattern in plants.

7.3.9. Relations between structural characteristics in rose bush and visual sensory attributes for objective evaluation of the visual quality

Participant: Jean-Baptiste Durand.

Joint work with: Gilles Galopin (QUASAV, Agrocampus Ouest)

Within ornamental horticulture context, visual quality of plants is a critical criterion for consumers looking for immediate decorative effect products. Studying links between architecture and its phenotypic plasticity in response to growing conditions and the resulting plant visual appearance represents an interesting lever to propose a new approach for managing product quality from specialized crops. Objectives of the present study were to determine whether architectural components may be identified across different growing conditions (1) to study the architectural development of a shrub over time; and (2) to predict sensory attributes data characterizing multiple visual traits of the plants. The approach addressed in this study stands on the sensory profile method using a recurrent blooming modern rose bush presented in rotation using video stimuli. Plants were cultivated under a shading gradient in three distinct environments (natural conditions, under 55% and 75% shading nets). Architecture and video of the plants were recorded during three stages, from 5 to 15 months after plant multiplication. Predictive models of visual quality were obtained with regression and variable transformation to encompass non-linear relationships [21]. The proposed approach is a way to gain a better insight into the architecture of shrub plants together with their visual appearance to target processes of interest in order to optimize growing conditions or select the most fitting genotypes across breeding programs, with respect to contrasted consumer preferences.

As a perspective, dynamic traits issued from hidden-Markov-based growth models should be used for a better characterization of visual quality, as well as identification of reiterated complexes, which are believed to play a major role in rose bush structure.

7.3.10. Bayesian neural networks

Participants: Julyan Arbel, Mariia Vladimirova.

Joint work with: Pablo Mesejo from University of Granada, Spain.

We investigate in [45] and [44] deep Bayesian neural networks with Gaussian priors on the weights and ReLU-like nonlinearities, shedding light on novel sparsity-inducing mechanisms at the level of the units of the network, both pre- and post-nonlinearities. The main thrust of the paper is to establish that the units prior distribution becomes increasingly heavy-tailed with depth. We show that first layer units are Gaussian, second layer units are sub-Exponential, and we introduce sub-Weibull distributions to characterize the deeper layers units. Bayesian neural networks with Gaussian priors are well known to induce the weight decay penalty on the weights. In contrast, our result indicates a more elaborate regularisation scheme at the level of the units. This result provides new theoretical insight on deep Bayesian neural networks, underpinning their natural shrinkage properties and practical potential.

MODAL Project-Team

7. New Results

7.1. Axis 1: 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 published in an international journal [12].

An extension of this work has been also presented to an international workshop.The idea is to use the data units principle as a way for (co-)clustering model enlargement.

It is a joint work with Alexandre Lourme from University of Bordeaux.

7.2. Axis 1: 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 now published in the international journal [18]. This is joint work Julien Jacques from University of Lyon 2.

7.3. Axis 1: 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 also be performed 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 is now under revision in an international journal [54] and has been presented to an international conference [38]. The related R package ordinalClust has been also written and has led to a specific preprint [57].

This is joint work with Margot Selosse (PhD student) and Julien Jacques, both from University of Lyon 2, and Florence Cousson-Gélie from University Paul Valéry Montpellier 3.

7.4. Axis 1: Model-based co-clustering for mixed type data

Participant: Christophe Biernacki.

Over decades, a lot of studies have shown the importance of clustering to emphasize groups of observations. More recently, due to the emergence of high-dimensional datasets with a huge number of features, co-clustering techniques have emerged and proposed several methods for simultaneously producing groups of observations and features. By synthesizing the dataset in blocks (the crossing of a row-cluster and a column-cluster), this technique can sometimes summarize better the data and its inherent structure. The Latent Block Model (LBM) is a well-known method for performing a co-clustering. However, recently, contexts with features of different types (here called mixed type datasets) are becoming more common. Unfortunately, the LBM is not directly applicable on this kind of dataset. The present work extends the usual LBM to the so-called Multiple Latent Block Model (MLBM) which is able to handle mixed type datasets. The inference is done through a Stochastic EM-algorithm embedding a Gibbs sampler and model selection criterion is defined to choose the number of row and column clusters. This method was successfully used on simulated and real datasets. This work is available as a preprint [55] which has been submitted to an international journal. It has also led to the R package mixedClust which has been presented to an international workshop [56] and has led to a specific preprint [56].

An adaptation of this general principle to the specific case of mixing textual and continuous data has been also proposed and presented to a national conference [26], with an international audience.

This is joint work with Margot Selosse (PhD student) and Julien Jacques, both from University of Lyon 2.

7.5. Axis 1: Model-Based Co-clustering with Co-variables

Participant: Serge Iovleff.

This work has been motivated by an epidemiological and genetic survey of malaria disease in Senegal. Data were collected between 1990 and 2008. It is based on a latent block model taking into account the problem of grouping variables and clustering individuals by integrating information given by a set of co-variables. Numerical experiments on simulated data sets and an application on real genetic data highlight the interest of this approach. BEM algorithm is deduced and implemented in R package *simerge* and has led to a specific preprint [24].

7.6. Axis 1: Relaxing the Identically Distributed Assumption in Gaussian Co-Clustering for High Dimensional Data

Participant: Christophe Biernacki.

A co-clustering model for continuous data that relaxes the identically distributed assumption within blocks of traditional co-clustering is presented. The proposed model, although allowing more flexibility, still maintains the very high degree of parsimony achieved by traditional co-clustering. A stochastic EM algorithm along with a Gibbs sampler is used for parameter estimation and an ICL criterion is used for model selection. Simulated and real datasets are used for illustr1ation and comparison with traditional co-clustering. This work has led to a preprint

This is a joint work with Michael Gallaugher (PhD student) and Paul Mcnicholas, both from McMaster University (Canada). Michael Gallaughter visited the Modal for three months in 2018.

7.7. Axis 1: Gaussian-based visualization of Gaussian and non-Gaussian model-based clustering

Participants: Christophe Biernacki, Vincent Vandewalle.

A generic method is introduced to visualize in a Gaussian-like way, and onto R^2, results of Gaussian or non-Gaussian model-based clustering. The key point is to explicitly force a spherical Gaussian mixture visualization to inherit from the within cluster overlap which is present in the initial clustering mixture. The result is a particularly user-friendly draw of the clusters, allowing any practitioner to have a thorough overview of the potentially complex clustering result. An entropic measure allows us to inform of the quality of the drawn overlap, in comparison to the true one in the initial space. The proposed method is illustrated on four real data sets of different types (categorical, mixed, functional and network) and is implemented on the R package ClusVis. This work has been submitted to an international journal [12] and has also been presented to an international conference [41].

This is a joint work with Matthieu Marbac from ENSAI.

7.8. Axis 1: A targeted multi-partitions clustering

Participants: Christophe Biernacki, Vincent Vandewalle.

Clustering is generally not a purpose by itself, because its results are mainly tools used by the statistician for another analysis. Indeed, in many applications, clusters are assessed from a set of observed variables, then these clusters are used to predict other variables which are used or not in clustering. Because the final objective of prediction is not considered during cluster analysis, there is no reason to obtain relevant clusters for the variables to predict. We present a unified approach which simultaneously performs cluster analysis and prediction. This method considers that the variables to clusters arise from a product of finite mixture models which provides multiple partition. Moreover, the variables to predict are considered to be independent of the variables to cluster given the partition. The predictions are achieved by a generalized linear model. Model selection is conducted by optimizing the BIC. This optimization is achieved with a modified version of the EM algorithm which performs model selection and maximum likelihood inference simultaneously. An early version of this work has been presented to an international conference [37].

It is a joint work with Matthieu Marbac from ENSAI and with Mohamed Sedki from Université Paris-Sud.

7.9. Axis 1: Co-clustering: A versatile way to perform clustering in high dimension

Participant: Christophe Biernacki.

Standard model-based clustering is known to be very efficient for low-dimensional data sets, but it fails for properly addressing high dimension (HD) ones, where it suffers from both statistical and computational drawbacks. In order to counterbalance this curse of dimensionality, some proposals have been made to take into account redundancy and features utility, but related models are not suitable for too many variables. We advocate that co-clustering, an unsupervised mixture model learning method to define simultaneously groups of rows (individuals) and groups of columns (variables) on a data matrix, is of particular interest to perform HD clustering of individuals even if it is not its primary mission. Indeed, column clustering is recast as a strategy to control the variance of the estimation, the model dimension being driven by the number of groups of variables instead of the number of variables itself. However, the statistical counterpart of this important variance reduction brings naturally some important model bias. The purpose is to access (first in an empirical manner) the trade-off bias-variance of the co-clustering strategy in scenarios involving HD fundaments (correlated variables, irrelevant variables). We show the ability of co-clustering to outperform simple mixture row-clustering, even if co-clustering clearly corresponds to a misspecified model situation, revealing a promising manner to efficiently address (very) HD clustering. An early version of this work has been presented to an international conference [36].

It is a joint work with Christine Keribin from Université Paris-Sud.

7.10. Axis 1: Dealing with missing data in model-based clustering through a MNAR model

Participants: Christophe Biernacki, Fabien Laporte.

Since the 90s, model-based clustering is largely used to classify data. Nowadays, with the increase of available data, missing values are more frequent. Traditional ways to deal with them consist in obtaining a filled data set, either by discarding missing values or by imputing them. In the first case, some information is lost; in the second case, the final clustering purpose is not taken into account through the imputation step. Thus, both solutions risk to blur the clustering estimation result. Alternatively, we defend the need to embed the missingness mechanism directly within the clustering modeling step. There exists three types of missing data: missing completely at random (MCAR), missing at random (MAR) and missing not at random (MNAR). In all situations logistic regression is proposed as a natural and flexible candidate model. In particular, its flexibility property allows us to design some meaningful parsimonious variants, as dependency on missing values or dependency on the cluster label. In this unified context, standard model selection criteria can be used to select between such different missing data mechanisms, simultaneously with the number of clusters. Practical interest of our proposal is illustrated on data derived from medical studies suffering from many missing data. An early version of this work has been presented to an international conference [33].

It is a joint work with Gilles Celeux from Inria Saclay and Julie Josse from Ecole Polytechnique.

7.11. Axis 1: Self Organizing Coclustering for textual data synthesis

Participant: Christophe Biernacki.

Recently, different studies have demonstrated the interest of co-clustering, which simultaneously produces clusters of lines and columns. The present work introduces a novel co-clustering model for parsimoniously summarizing textual data in documents × terms format. Besides highlighting homogeneous coclusters - as other existing algorithms do - we also distinguish noisy coclusters from significant ones, which is particularly useful for sparse documents × term matrices. Furthermore, our model proposes a structure among the significant coclusters and thus obtains a better interpretability to the user. By forcing a structure through row-clusters and column-clusters, this approach is competitive in terms of documents clustering, and offers user-friendly results. The algorithm derived for the proposed method is a Stochastic EM algorithm embedding a Gibbs sampling step and the Poisson distribution. A preprint is currently in progress.

This is joint work with Margot Selosse (PhD student) and Julien Jacques, both from University of Lyon 2.

7.12. Axis 1: Linking canonical and spectral clustering

Participants: Christophe Biernacki, Vincent Vandewalle.

It is a recent work aiming at defining a mathematical bridge between classical model-based clustering and classical spectral clustering. Interest of such a prospect is to be able to compare both methods through the rigorous scheme of model selection paradigm. It is an ongoing work.

It is a joint work with Alexandre Lourme from University of Bordeaux.

7.13. Axis 1: Multiple partition clustering

Participant: Vincent Vandewalle.

In the framework of model-based clustering, a model allowing several latent class variables have been proposed. This model assumes that the distribution of the observed data can be factorized into several independent blocks of variables. Each block is assumed to follow a latent class model (i.e., mixture with conditional independence assumption). The proposed model includes variable selection, as a special case, and is able to cope with the mixed-data setting. The simplicity of the model allows to estimate the repartition of the variables into blocks and the mixture parameters simultaneously, thus avoiding running EM algorithms for each possible repartition of variables into blocks. For the proposed method, a model is defined by the number of blocks, the number of clusters inside each block and the repartition of variables into blocks. Model selection can be done with two information criteria, the BIC and the MICL, for which an efficient optimization is proposed. The proposed method gives a rich interpretation of the data set at hand (i.e., analysis of the repartition of the variables into blocks and analysis of the clusters produced by each block of variables). This work as been presented in several international conferences and is now published [20].

It is a joint work with Matthieu Marbac from ENSAI.

7.14. Axis 2: Change-point detection by means of reproducing kernels

Participant: Alain Celisse.

Classical offline change-point detection approaches are limited to detecting changes arising in the mean and/or variance of the distribution along the time. Detecting changes in other moments of the distribution is possible, but at the price of stronger (unrealistic) distributional assumptions which are likely to be violated.

Reproducing kernels are a means to detect changes arising in any moments of the distribution along the time, which are not limited to the mean or the variance. One of the main contributions of this work is to provide a theoretically grounded model selection strategy allowing us to detection multiple changes. From additional extensive simulation experiments, it clearly arises that the so-called KCP approach outperforms numerous state-of-the art change-points detection procedures such as E-divisive, PELT, ...

7.15. Axis 2: New efficient algorithms for multiple change-point detection with kernels

Participants: Alain Celisse, Guillemette Marot.

Several statistical approaches based on reproducing kernels have been proposed to detect abrupt changes arising in the full distribution of the observations and not only in the mean or variance. Some of these approaches enjoy good statistical properties (oracle inequality, ...). Nonetheless, they have a high computational cost both in terms of time and memory. This makes their application difficult even for small and medium sample sizes ($n < 10^4$). This computational issue is addressed by first describing a new efficient and exact algorithm for kernel multiple change-point detection with an improved worst-case complexity that is quadratic in time and linear in space. It allows dealing with medium size signals (up to $n \approx 10^5$). Second, a faster but approximation algorithm is described. It is based on a low-rank approximation to the Gram matrix. It is linear in time and space. This approximation algorithm can be applied to large-scale signals ($n \geq 10^6$). These exact and approximation algorithms have been implemented in `R` and `C` for various kernels. The computational and statistical performances of these new algorithms have been assessed through empirical experiments. The runtime of the new algorithms is observed to be faster than that of other considered procedures. Finally, simulations confirmed the higher statistical accuracy of kernel-based approaches to detect changes that are not only in the mean. These simulations also illustrate the flexibility of kernel-based approaches to analyze complex biological profiles made of DNA copy number and allele B frequencies. An R package implementing the approach will be made available on github.

7.16. Axis 2: Multi-Layer Group-Lasso

Participants: Alain Celisse, Guillemette Marot.

Multi-Layer Group-Lasso (MLGL) is a new procedure of variable selection in the context of redundancy between explanatory variables, which holds true with high-dimensional data. A sparsity assumption is made that is, only a few variables are assumed to be relevant for predicting the response variable. In this context, the performance of classical Lasso-based approaches strongly deteriorate as the redundancy strengthens. The proposed approach combines variable aggregation and selection in order to improve interpretability and performance. First, a hierarchical clustering procedure provides at each level a partition of the variables into groups. Then, the set of groups of variables from the different levels of the hierarchy is given as input to group-Lasso, with weights adapted to the structure of the hierarchy. At this step, group-Lasso outputs sets of candidate groups of variables for each value of regularization parameter. The versatility offered by MLGL to choose groups at different levels of the hierarchy a priori induces a high computational complexity. MLGL however exploits the structure of the hierarchy and the weights used in group-lasso to greatly reduce the final time cost. The final choice of the regularization parameter – and therefore the final choice of groups – is made by a multiple hierarchical testing procedures. A paper associated to the R package MLGL has been submitted [45].

7.17. Axis 2: Pseudo-Bayesian Learning with Kernel Fourier Transform as Prior

Participants: Pascal Germain, Gael Letarte.

We revisit the kernel random Fourier features (RFF) method through the lens of the PAC-Bayesian theory. While the primary goal of RFF is to approximate a kernel, we look at the Fourier transform as a prior distribution over trigonometric hypotheses. It naturally suggests learning a posterior on these hypotheses. We derive generalization bounds that are optimized by learning a pseudo-posterior obtained from a closed-form expression, and corresponding learning algorithms This work has been accepted for publication at AISTATS 2019 conference [51].

It is a joint work with Emilie Morvant from Université Jean Monnet de Saint-Etienne.

7.18. Axis 2: Decentralized learning with budgeted network load using Gaussian copulas and classifier ensembles

Participant: Benjamin Guedj.

We examine a network of learners which address the same classification task but must learn from different data sets. The learners can share a limited portion of their data sets so as to preserve the network load. We introduce DELCO (standing for Decentralized Ensemble Learning with COpulas), a new approach in which the shared data and the trained models are sent to a central machine that allows to build an ensemble of classifiers. The proposed method aggregates the base classifiers using a probabilistic model relying on Gaussian copulas. Experiments on logistic regressor ensembles demonstrate competing accuracy and increased robustness as compared to gold standard approaches. A companion python implementation can be downloaded at https://github.com/john-klein/DELCO.

Joint work with John Klein, Olivier Colot, Mahmoud Albardan (all from CRIStAL lab, UMR 9189, Univ. Lille. Preprint submitted: [50].

7.19. Axis 2: Sequential Learning of Principal Curves: Summarizing Data Streams on the Fly

Participants: Benjamin Guedj, Le Li.

When confronted with massive data streams, summarizing data with dimension reduction methods such as PCA raises theoretical and algorithmic pitfalls. Principal curves act as a nonlinear generalization of PCA and the present paper proposes a novel algorithm to automatically and sequentially learn principal curves from data streams. We show that our procedure is supported by regret bounds with optimal sublinear remainder terms. A greedy local search implementation that incorporates both sleeping experts and multi-armed bandit ingredients is presented, along with its regret bound and performance on a toy example and seismic data.

Preprint submitted: [47].

7.20. Axis 2: A Quasi-Bayesian Perspective to Online Clustering

Participants: Benjamin Guedj, Le Li.

When faced with high frequency streams of data, clustering raises theoretical and algorithmic pitfalls. We introduce a new and adaptive online clustering algorithm relying on a quasi-Bayesian approach, with a dynamic (i.e., time-dependent) estimation of the (unknown and changing) number of clusters. We prove that our approach is supported by minimax regret bounds. We also provide an RJMCMC-flavored implementation (called PACBO, see https://cran.r-project.org/web/packages/PACBO/index.html) for which we give a convergence guarantee. Finally, numerical experiments illustrate the potential of our procedure.

Joint work with Sébastien Loustau (LumenAI). Paper published in Electronic Journal of Statistics: https://projecteuclid.org/euclid.ejs/1537430425, [19].

7.21. Axis 2: Pycobra: A Python Toolbox for Ensemble Learning and Visualisation

Participants: Benjamin Guedj, Bhargav Srinivasa Desikan.

We introduce pycobra, a Python library devoted to ensemble learning (regression and classification) and visualisation. Its main assets are the implementation of several ensemble learning algorithms, a flexible and generic interface to compare and blend any existing machine learning algorithm available in Python libraries (as long as a predict method is given), and visualisation tools such as Voronoi tessellations. pycobra is fully scikit-learn compatible and is released under the MIT open-source license. pycobra can be downloaded from the Python Package Index (PyPi) and Machine Learning Open Source Software (MLOSS). The current version (along with Jupyter notebooks, extensive documentation, and continuous integration tests) is available at https://github.com/bhargavvader/pycobra and official documentation website is https://modal.lille.inria.fr/pycobra.

Paper published in Journal of Machine Learning Research: http://jmlr.org/papers/v18/17-228.html, [17]. Software submitted to the `scikit-learn-contrib` repository (under review).

7.22. Axis 2: Simpler PAC-Bayesian bounds for hostile data

Participant: Benjamin Guedj.

PAC-Bayesian learning bounds are of the utmost interest to the learning community. Their role is to connect the generalization ability of an aggregation distribution ρ to its empirical risk and to its Kullback-Leibler divergence with respect to some prior distribution π. Unfortunately, most of the available bounds typically rely on heavy assumptions such as boundedness and independence of the observations. This paper aims at relaxing these constraints and provides PAC-Bayesian learning bounds that hold for dependent, heavy-tailed observations (hereafter referred to as hostile data). In these bounds the Kullack-Leibler divergence is replaced with a general version of Csiszár's f-divergence. We prove a general PAC-Bayesian bound, and show how to use it in various hostile settings.

Joint work with Pierre Alquier (ENSAE ParisTech). Paper published in Machine Learning: [11].

7.23. Axis 2: PAC-Bayesian high dimensional bipartite ranking

Participant: Benjamin Guedj.

This paper is devoted to the bipartite ranking problem, a classical statistical learning task, in a high dimensional setting. We propose a scoring and ranking strategy based on the PAC-Bayesian approach. We consider nonlinear additive scoring functions, and we derive non-asymptotic risk bounds under a sparsity assumption. In particular, oracle inequalities in probability holding under a margin condition assess the performance of our procedure, and prove its minimax optimality. An MCMC-flavored algorithm is proposed to implement our method, along with its behavior on synthetic and real-life datasets.

Joint work with Sylvain Robbiano. Paper published in Journal of Statistical Planning and Inference: [16].

7.24. Axis 2: Multiview Boosting by Controlling the Diversity and the Accuracy of View-specific Voters

Participant: Pascal Germain.

We propose a boosting based multiview learning algorithm which iteratively learns i) weights over view-specific voters capturing view-specific information; and ii) weights over views by optimizing a PAC-Bayes multiview C-Bound that takes into account the accuracy of view-specific classifiers and the diversity between the views. We derive a generalization bound for this strategy following the PAC-Bayes theory which is a suitable tool to deal with models expressed as weighted combination over a set of voters. This work has been submitted to an international journal and is available as a preprint [44].

It is a joint work with Emilie Morvant from Université Jean Monnet de Saint-Etienne and with Massih-Reza Amini of Université de Grenoble, and with Anil Goyal affiliated to both institutions.

7.25. Axis 3: Clustering spatial functional data

Participants: Sophie Dabo, Cristian Preda, Vincent Vandewalle.

We propose two approaches for clustering spatial functional data. The first one is the model-based clustering that uses the concept of density for functional random variables. The second one is the hierarchical clustering based on univariate statistics for functional data such as the functional mode or the functional mean. These two approaches take into account the spatial features of the data: two observations that are spatially close share a common distribution of the associated random variables. The two methodologies are illustrated by an application to air quality data. This work will appear in the "Geostatistical Functional Data Analysis: Theory and Methods". Wiley, 2018. Editors : Jorge Mateu, Ramon Giraldo [39].

7.26. Axis 3: Categorical functional data analysis

Participants: Cristian Preda, Vincent Vandewalle.

We develop and implement techniques for analysis of categorical functional data. Visualization, clustering and regression methods with categorical functional predictor are proposed.

7.27. Axis 4: Real-time Audio Sources Classification

Participants: Christophe Biernacki, Maxime Baelde.

This work addresses the recurring challenge of real-time monophonic and polyphonic audio source classification. The whole power spectrum is directly involved in the proposed process, avoiding complex and hazardous traditional feature extraction. It is also a natural candidate for polyphonic events thanks to its additive property in such cases. The classification task is performed through a nonparametric kernel-based generative modeling of the power spectrum. Advantage of this model is twofold: it is almost hypothesis free and it allows to straightforwardly obtain the maximum a posteriori classification rule of online signals. Moreover it makes use of the monophonic dataset to build the polyphonic one. Then, to reach the real-time target, the complexity of the method can be tuned by using a standard hierarchical clustering preprocessing of sound models, revealing a particularly efficient computation time and classification accuracy trade-off. The proposed method reveals encouraging results both in monophonic and polyphonic classification tasks on benchmark and owned datasets, even in real-time situations. This method also has several advantages compared to the state-of-the-art methods include a reduced training time, no hyperparameters tuning, the ability to control the computation - accuracy trade-off and no training on already mixed sounds for polyphonic classification. This work is now under revision to an international journal [40].

It is a joint work with Raphaël Greff, from the A-Volute company.

7.28. Axis 4: Matching of descriptors evolving over time

Participants: Christophe Biernacki, Anne-Lise Bedenel.

In the web domain, and in particular for insurance comparison, data constantly evolve, implying that it is difficult to directly exploit them. For example, to do a classification, performing standard learning processes require data descriptors equal for both learning and test samples. Indeed, for answering web surfer expectation, online forms whence data come from are regularly modified. So, features and data descriptors are also regularly modified. In this work, it is introduced a process to estimate and understand connections between transformed data descriptors. This estimated matching between descriptors will be a preliminary step before applying later classical learning methods. This work has been presented to a national conference [27], with an international audience, and also to an international conference [28].

It is a joint work with Laetitia Jourdan, from University of Lille.

7.29. Axis 4: Supervised multivariate discretization and levels merging for logistic regression

Participants: Christophe Biernacki, Vincent Vandewalle, Adrien Ehrhardt.

For regulatory and interpretability reasons, the logistic regression is still widely used by financial institutions to learn the refunding probability of a loan given the applicants characteristics from historical data. Although logistic regression handles naturally both quantitative and qualitative data, three ad hoc pre-processing steps are usually performed: firstly, continuous features are discretized by assigning factor levels to predetermined intervals; secondly, qualitative features, if they take numerous values, are grouped; thirdly, interactions (products between two different features) are sparsely introduced. By reinterpreting these discretized (resp. grouped) features as latent variables and by modeling the conditional distribution of each of these latent variables given each original feature with a polytomous logistic link (resp. contingency table), a novel model-based resolution of the discretization problem is introduced. Estimation is performed via a Stochastic Expectation-Maximization (SEM) algorithm and a Gibbs sampler to find the best discretization (resp. grouping) scheme w.r.t. any classical logistic regression loss (AIC, BIC, test set AUC, ...). For detecting interacting features, the same scheme is used by replacing the Gibbs sampler by a Metropolis-Hastings algorithm. The good performances of this approach are illustrated on simulated and real data from Credit Agricole Consumer Finance. This work has been presenting to an international conference in statistics [35] and has been also submitting to an international conference in machine learning. [42].

This is a joint work with Philippe Heinrich from University of Lille.

7.30. Axis 4: MASSICCC Platform for SaaS Software Availability

Participant: Christophe Biernacki.

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 (forMixmod,MixtComp and BlockCluster) directly in the web platform itself has led to some specific developments. In 2018, MASSICCC has been presented to a workshop [29]. Currently, a preprint for an international journal dedicated to software is also in progress.

The MASSICCC platform is available here in the web: https://massiccc.lille.inria.fr.

7.31. Axis 4: ClinMine: Optimizing the Management of Patients in Hospital

Participants: Cristian Preda, Vincent Vandewalle.

A better understanding of “patient pathway” thanks to data analysis can lead to better treatments for patients. The ClinMine project, supported by the French National Research Agency (ANR), aims at proposing, from various case studies, algorithmic and statistical models able to handle this type of pathway data, focusing primarily on hospital data.

Case studies, focusing on the integration of temporal data within analysis has been published [14]. First, the hypothesis that some aspects of the patient pathway can be described, even predicted, from the management process of the hospital medical mail is studied. Therefore a specific functional data analysis is driven, and several types of patients have been detected. The second case study deals with the detection of profiles through a biclustering of the patients. The difficulty to simultaneously deal with heterogeneous data, including temporal data is exposed and a method is proposed.

7.32. Projection Under Pairwise Control

Participant: Christophe Biernacki.

Visualization of high-dimensional and possibly complex (non-continuous for instance) data onto a low-dimensional space may be difficult. Several projection methods have been already proposed for displaying such high-dimensional structures on a lower-dimensional space, but the information lost is not always easy to use. Here, a new projection paradigm is presented to describe a non-linear projection method that takes into account the projection quality of each projected point in the reduced space, this quality being directly available in the same scale as this reduced space. More specifically, this novel method allows a straightforward visualization data in R2 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 [48].

It is a joint work with Hiba Alawieh and Nicolas Wicker, both from University of Lille.

RANDOPT Team

7. New Results

7.1. Analysis of adaptive Stochastic Optimizers

7.1.1. New ODE method for proving the geometric convergence of adaptive Stochastic Optimizers

The ODE method is a standard technique to analyze the convergence of stochastic algorithms defined as a stochastic approximation of an ODE. In a nutshell, the convergence of the algorithms derives from the stability of the ODE and the control of the error between the solution of the ODE and the trajectory of the stochastic algorithm. We have been developing a new ODE method to be able to prove the geometric convergence of stochastic approximation algorithms that derive from the family of adaptive stochastic optimization algorithms. Standard theory did not apply in this context as the state variable adapted typically converge to the boundary of the state-space domain where an infinite number of points are equilibrium points for the ODE [7].

7.1.2. Convergence and convergence rate analysis of the (1+1)-ES with one-fifth success rule

When analyzing adaptive stochastic optimizers, one is typically interested to prove the linear convergence and investigate the dependency of the convergence rate with respect to the dimension. We have greatly simplified the analysis of the convergence and convergence rate of the (1+1)-ES with one-fifth success rule on the sphere function. We have shown that the analysis derives from applying a simple "drift" theorem and consequently shown a hitting time to reach an ϵ-ball of the optimum of $\Theta(\frac{1}{d}\log(1/\epsilon))$ akin to linear convergence with a convergence rate scaling linearly with the dimension [4].

7.1.3. Quality-gain Analysis on Convex-quadratic functions

We have analyzed the expected function value decrease (related to the convergence rate) of Evolution Strategies with weighed recombination on convex-quadratic functions. We have derive different bounds and limit expression that allow to derive optimal recombination weights and the optimal step-size, and found that the optimal recombination weights are independent of the Hessian of the objective function. We have moreover shown the dependencies of the optimal parameters in the dimension and population size [1].

7.2. Benchmarking Methodology

7.2.1. Single-Objective Benchmarking

Benchmarking optimization algorithms seems trivial at first sight but is quite involved in practice and little decisions on the experimental setup can have a large effect on the displayed algorithm performance.

We have investigated some of these effects in the context of the Black-Box Optimization Benchmarking (`bbob`) test suite of the COCO platform and the well-known quasi-Newton BFGS algorithm, default in MATLAB's `fminunc` and in Python's `scipy.optimize` module [5]. We realized in particular that the instance instantiation in the COCO platform has little impact while the initial search point has a larger one. The largest performance differences, however, stem from implementation details that are typically not documented and not exposed to the user via internal algorithm parameters. For example is the MATLAB implementation of the BFGS algorithm significantly worse than the Python implementation and the MATLAB 2017 version is worse than the MATLAB 2009 implementation.

Additionally, Nikolaus Hansen gave a hands-on tutorial on good benchmarking practice at the GECCO-2018 conference in Kyoto [11].

7.2.2. Multi-Objective Benchmarking

In terms of multiobjective benchmarking, our contributions are two-fold. Firstly, we wrote a scientific article on the scientific methodology for defining our new multiobjective benchmark suite. In [10] we introduce two new bi-objective test suites on the basis of the above mentioned, well-known 24 `bbob` test functions and propose a generic test suite generator for an arbitrary number of objectives. The former are implemented in our COCO platform and extensively documented in terms of search and objective space plots for each function.

Secondly, we realized with the proposal of the biobjective `bbob` test suites that there is a need for more theoretical analyses of simple test functions that still test for practical challenges such as ill-conditioning or search space rotations. In our upcoming EMO conference paper [3] we therefore characterize theoretically Pareto sets and Pareto fronts of combinations of two convex quadratic functions with arbitrary search space dimension. Based on this theoretical analysis, we suggest a wide set of new biobjective test functions.

7.3. Large-scale Optimization

We have been studying different large-scale variants of the CMA-ES algorithm and tested them thoroughly empirically on a set of scalable large-scale testbed. The study includes comparison with the large-scale quasi-Newton algorithm, namely L-BFGS [6].

7.4. Constrained Optimization

In the context of constrained optimization, A. Atamna studied invariance properties of Augmented Lagrangian approaches and showed the relation between invariance to strictly increasing affine transformations of the objective function and the scaling of the constraints and linear convergence [2]. Progress were made towards a methodology to define scalable constrained problems with control optimum and the implementation of a new constrained testbed within the COCO platform. In her internship, E. Marescaux studied the connection between augmented Lagrangian approaches and a previously proposed adaptive constrained handling mechanism. She also studied a new idea to turn a constrained problem into an unconstrained one.

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 [6] 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 [8] 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. Routing Problems

In [7] 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.

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 [5] 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.

We examined the robust counterpart of the classical Capacitated Vehicle Routing Problem (CVRP) in [13], [20]. We considered two types of uncertainty sets for the customer demands: the classical budget polytope introduced by Bertsimas and Sim (2003), and a partitioned budget polytope proposed by Gounaris et al. (2013). We showed that using the set-partitioning formulation it is possible to reformulate our problem as a deterministic heterogeneous vehicle routing problem. Thus, many state-of-the-art techniques for exactly solving deterministic VRPs can be applied for the robust counterpart, and a modern branch-and-cut-and-price algorithm can be adapted to our setting by keeping the number of pricing subproblems strictly polynomial. More importantly, we introduced new techniques to significantly improve the efficiency of the algorithm. We present analytical conditions under which a pricing subproblem is infeasible. This result is general and can be applied to other combinatorial optimization problems with knapsack uncertainty. We also introduced robust capacity cuts which are provably stronger than the ones known in the literature. Finally, a fast iterated local search algorithm was proposed to obtain heuristic solutions for the problem. Using our branch-and-cut-and-price algorithm incorporating existing and new techniques, we were able to solve to optimality all but one open instances from the literature.

In [14], we have generalized our Branch-Cut-and-Price algorithm to solve other Vehicle Routing and related combinatorial optimization problems, as Generalized Assignment, Bin Packing, and Vector Packing. Our generic approach outperformed several problem specific algorithms.

7.3. Scheduling and Clustering Problems

In [19] 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.

A cross-docking terminal is a transshipment facility in supply chains, where products transported by inbound trucks are unloaded at inbound doors, sorted, and reloaded on outbound trucks at outbound doors. In [16], we address the truck-to-door scheduling problem at a multi-door cross-docking terminal where temporary storage is considered. We propose two types of time-indexed formulation for the problem to assign trucks to dock doors and determine their arrival and departure times so that tadiness and earliness as well as unsatisfied demand are minimized. We examine the effectiveness of the proposed formulations by numerical experiment.

7.4. Scheduling and placement for HPC

In High Performance Computing, heterogeneity is now the norm with specialized accelerators like GPUs providing efficient computational power. Resulting complexity led to the development of task-based runtime systems, where complex computations are described as task graphs, and scheduling decisions are made at run-time to perform load balancing between all resources of the platforms. In [2], we consider the problem of developing good scheduling strategies, even at the scale of a single node, and analyzing them both theoretically and in practice is expected to have a very high impact on the performance of current HPC systems. The special case of two kinds of resources, typically CPUs and GPUs is already of great practical interest. The scheduling policy Hetero-Prio has been proposed in the context of fast multipole computations (FMM), and has been

extended to general task graphs with very promising results. In this paper, we provide a theoretical study of the performance of HeteroPrio, by proving approximation bounds compared to the optimal schedule, both in the case of independent tasks and in the case of general task graphs. Interestingly, our results establish that spoliation (a technique that enables resources to restart uncompleted tasks on another resource) is enough to prove bounded approximation ratios for a list scheduling algorithm on two unrelated resources, which is known to be impossible otherwise. This result holds true both for independent and dependent tasks graphs. Additionally, we provide an experimental evaluation of HeteroPrio on real task graphs from dense linear algebra computation, that establishes its strong performance in practice.

In [1], we consider the problem of partitioning a matrix into a set of sub-matrices, that 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 preexisting 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 analyze how close to the known optimal solutions the NRRP algorithm is for small numbers of partitions.

In [12], we consider the problem of data allocation 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.

7.5. Convergence between HPC and Data Science

In [11] paper we concentrate on a crucial parameter for efficiency in Big Data and HPC applications: data locality. We focus on the scheduling of a set of independent tasks, each depending on an input file. We assume that each of these input files has been replicated several times and placed in local storage of different nodes of a cluster, similarly of what we can find on HDFS system for example. We consider two optimization problems, related to the two natural metrics: makespan optimization (under the constraint that only local tasks are allowed) and communication optimization (under the constraint of never letting a processor idle in order to optimize makespan). For both problems we investigate the performance of dynamic schedulers, in particular the basic greedy algorithm we can for example find in the default MapReduce scheduler. First we theoretically study its performance, with probabilistic models, and provide a lower bound for communication metric and asymptotic behaviour for both metrics. Second we propose simulations based on traces from a Hadoop cluster to compare the different dynamic schedulers and assess the expected behaviour obtained with the theoretical study.

In [10], we consider the use of Burst-Buffers, that 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.

7.6. Energy management

In [9], we consider energy management optimization problems in a future wherein an interaction with micro-grids has to be accounted for. We model this interaction through a set of contracts between the generation companies owning centralized assets and the micro-grids. We formulate a general stylized model that can, in principle, account for a variety of management questions such as unit-commitment. The resulting model, a bilevel stochastic mixed integer program will be numerically tackled through a novel preprocessing procedure. As a result the solution for the bilevel (or single leader multiple follower) problem will be neither " optimistic " nor " pessimistic ". We numerically evaluate the difference of the resulting solution with the " optimistic " solution. We also demonstrate the efficiency and potential of our methodology on a set of numerical instances.

7.7. Network Design Problems

The delivery of freight from manufacturing platforms to demand zones is often managed through one or more intermediate locations where storing, merging, transshipment and consolidation activities are performed. In [56], 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.

In [33], we study the k-edge-connected L-hop-constrained network design problem. Given a weighted graph $G = (V, E)$, a set D of pairs of nodes, two integers $L \geq 2$ and $k \geq 2$, the problem consists in finding a minimum weight subgraph of G containing at least k edge-disjoint paths of length at most L between every pair $\{s, t\} \in D$. We consider the problem in the case where $L = 2$, 3 and $|D| \geq 2$. We first discuss integer programming formulations introduced in the literature. Then, we introduce new integer programming formulations for the problem that are based on the transformation of the initial undirected graph into directed layered graphs. We present a theoretical comparison of these formulations in terms of LP-bound. Finally, these formulations are tested using CPLEX and compared in a computational study for $k = 3, 4, 5$.

In [72], we consider a multi-layer network design model arising from a real-life telecommunication application where traffic routing decisions imply the installation of expensive nodal equipment. Customer requests come in the form of bandwidth reservations for a given origin destination pair. Bandwidth demands are expressed as multiples of nominal granularities. Each request must be single-path routed. Grooming several requests on the same wavelength and multiplexing wavelengths in the same optical stream allow a more efficient use of network capacity. However, each addition or withdrawal of a request from a wavelength requires optical to electrical conversion and the use of cross-connect equipment with expensive ports of high densities. The objective is to minimize the number of required ports of the cross-connect equipment. We deal with backbone optical networks, therefore with networks with a moderate number of nodes (14 to 20) but thousands of requests. Further difficulties arise from the symmetries in wavelength assignment and traffic loading. Traditional multi-commodity network flow approaches are not suited for this problem. Instead, four alternative models relying on Dantzig-Wolfe and/or Benders' decomposition are introduced and compared. The formulations are strengthened using symmetry breaking restrictions, variable domain reduction, zero-one discretization of integer variables, and cutting planes. The resulting dual bounds are compared to the values of primal solutions obtained through hierarchical optimization and rounding procedures. For realistic size instances, our best approaches provide solutions with optimality gap of approximately 5% on average in around two hours of computing time.

7.8. Packing and 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 [3], 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 [21] 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.

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.

In collaboration with Damien Garreau, Sylvain Arlot studied the kernel change-point algorithm (KCP) proposed by Arlot, Celisse and Harchaoui (2012), which aims at locating an unknown number of change-points in the distribution of a sequence of independent data taking values in an arbitrary set. The change-points are selected by model selection with a penalized kernel empirical criterion. We provide a non-asymptotic result showing that, with high probability, the KCP procedure retrieves the correct number of change-points, provided that the constant in the penalty is well-chosen; in addition, KCP estimates the change-points location at the optimal rate. As a consequence, when using a characteristic kernel, KCP detects all kinds of change in the distribution (not only changes in the mean or the variance), and it is able to do so for complex structured data (not necessarily in Rd). Most of the analysis is conducted assuming that the kernel is bounded; part of the results can be extended when we only assume a finite second-order moment.

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 Benjamin Charlier and Jean-Michel Marin (Université de Montpellier), Gilles Celeux has started research aiming to propose a rapid Bayesian algorithm to estimate simply the mode of a posterior distribution for hidden structure models. This Bayesian procedure is of interest for two reasons. First, it leads to regularised estimation, which is useful for poorly posed problems. Second, it is an interesting alternative to variational approximation.

6.2. Estimator selection and statistical tests

Participant: Sylvain Arlot.

Sylvain Arlot wrote a book chapter about cross-validation in 2018. This text defines all classical cross-validation procedures, and studies their properties for two different goals: estimating the risk of a given estimator, and selecting the best estimator among a given family. For the risk estimation problem, it computes the bias (which can also be corrected) and the variance of cross-validation methods. For estimator selection, it first provides a first-order analysis (based on expectations). Then, it explains how to take into account second-order terms (from variance computations, and by taking into account the usefulness of over-penalization). This allows, in the end, to provide some guidelines for choosing the best cross-validation method for a given learning problem.

6.3. Statistical learning methodology and theory

Participants: Gilles Celeux, Serge Cohen, Christine Keribin, Michel Prenat, Sylvain Arlot, Benjamin Auder, Jean-Michel Poggi, Neska El Haouij, Kevin Bleakley, Matthieu Lerasle.

Sylvain Arlot wrote a book chapter about supervised statistical learning, from the mathematical point of view in 2018. This text describes the general prediction problem and the two key examples of regression and binary classification. Then, it studies two kinds of learning rules: empirical risk minimizers, which naturally lead to convex risks in classification, and local averaging rules, for which a universal consistency result can be obtained. Finally, it identifies the limits of learning in order to underline its challenges. The text ends with some useful probabilistic tools and some exercises.

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 χ^2 distance, while spatial homogeneity is associated with a single link distance. This year they have developed a hybrid hierarchical clustering procedure in which sub-clusters respecting spatial consistency are constructed. Then, these sub-clusters are merged without taking spatial constraints into account. This strategy leads to a more realistic segmentation of spectral images.

Gilles Celeux continued his collaboration with Jean-Patrick Baudry on model-based clustering. Last 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. This year, this work was completed, and performed well in comparison with state-of-the-art procedures.

Gillies Celeux has continued research on missing data for model-based clustering in collaboration with Christophe Biernacki (Modal team, Inria Lille) and Julie Josse (École Polytechnique). This year, they implemented several algorithms to estimate their logistic 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.It leads to a simple procedure to represent the proximity between clusters without any additional assumptions.

After having proved the consistency and asymptotic normality of Latent Block Model estimators with V. Brault and M. Mariadassou, Christine Keribin has worked on the behavior of the ICL and BIC model criteria in this model, and in particular on their probable asymptotic equivalence.

Christine Keribin has started a new collaboration with Christophe Biernacki (Inria Modal Team) to study the ability for co-clustering to be a good regularized method for clustering in HD, which was presented at the CMStatistics 2018 conference.

J-M. Poggi (with R. Genuer), published a survey paper dedicated to “Arbres CART et Forêts aléatoires, Importance et sélection de variables”, as a book chapter published in: “Apprentissage Statistique et Données Massives” by Technip.

J.-M. Poggi and N. El Haouij (with R. Ghozi, S. Sevestre Ghalila and M. Jaïdane) provide a random forest-based method for the selection of physiological functional variables in order to classify the stress level during real-world driving experience. The contribution of this study is twofold: on the methodological side, it considers physiological signals as functional variables and offers a procedure of data processing and variable selection. On the applied side, the proposed method provides a “blind” procedure of driver’s stress level classification that does not depend on the expert-based studies of physiological signals. This work has been published in Statistical Methods & Applications.

J.-M. Poggi and N. El Haouij (with R. Ghozi, S. Sevestre Ghalila and M. Jaïdane provide a system and database to assess driver’s attention, called aAffectiveROAD. A paper presenting it has been published in the proceedings of the 33rd ACM Symposium on Applied Computing SAC’18.

6.4. Statistical analysis of genomic data

Participant: Kevin Bleakley.

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 on this was published in the Journal of Infectious Diseases in 2018.

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 was published in the FASEB journal in 2018.

Kevin Bleakley worked as part of a consortium on a crowdsourced Dream Challenge in 2018 on using molecular signatures to predict susceptibility to viral infection. Essentially, many teams of researchers from around the world used machine learning (statistical learning) algorithms to learn on training data then test on unseen real data. In the final stage, methods from several teams were combined to improve overall prediction performance. The article "A crowdsourced analysis to identify ab initio molecular signatures predictive of susceptibility to viral infection" was published in Nature Communications in 2018.

6.5. Reliability

Participants: Gilles Celeux, Florence Ducros, Patrick Pamphile.

From June 2015 until June 2018 when she defended it, in the framework of a CIFRE convention with Nexter, Florence Ducros researched 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. Dynamical systems

Participant: Sylvain Arlot.

In collaboration with Stefano Marmi and Duccio Papini, Sylvain Arlot proposed a new model for the time evolution of livestock commodities which exhibits endogenous deterministic stochastic behaviour. The model is based on the Yoccoz-Birkeland integral equation, a model first developed for studying the time-evolution of single species with high average fertility, a relatively short mating season and density dependent reproduction rates. This equation is then coupled with a differential equation describing the price of a livestock commodity driven by the unbalance between its demand and supply. At its birth the cattle population is split into two parts: reproducing females and cattle for butchery. The relative amount of the two is determined by the spot price of the meat. We prove the existence of an attractor and we investigate numerically its properties: the strange attractor existing for the original Yoccoz-Birkeland model is persistent but its chaotic behaviour depends also from the price evolution in an essential way.

6.7. Soccer forecasting

Participants: Gilles Celeux, Jean-Louis Foulley.

In collaboration with Jean-Louis Foulley (Montpellier University), Gilles Celeux has proposed a penalty criterion for assessing correct score forecasting in soccer matches. They have defined the subject of a Masters internship for next year to predict scores of soccer matches via Poisson models using maximum likelihood and Bayesian inference.

6.8. Electricity load forecasting and clustering

Participants: Jean-Michel Poggi, Benjamin Auder, Benjamin Goehry.

B. Auder, J-M. Poggi (with J. Cugliari, Y. Goude) are interested in hierarchical time-series for bottom-up forecasting. The idea is to disaggregate the signal in such a way that the sum of disaggregated forecasts improves the direct prediction. The 3-steps strategy defines numerous super-consumers by curve clustering, builds a hierarchy of partitions and selects the best one minimizing a forecast criterion. Using a nonparametric model to handle forecasting, and wavelets to define various notions of similarity between load curves, this disaggregation strategy applied to French individual consumers leads to a gain of 16% in forecast accuracy. Then the upscaling capacity of this strategy facing massive data is explored and different proposals using R are experimented. The proposed solutions to make the algorithm scalable combines data storage, parallel computing and double clustering step to define the super-consumers. This has been published in the journal Energies.

Benjamin Goehry is completing a thesis co-supervised by P. Massart and J-M. Poggi, aiming at extending this scheme by introducing the use of random forests as time series forecasting models adapted to each cluster.

J.-M. Poggi (with J. Cugliari) published in Wiley StatsRef-Statistics Reference Online, a paper entitled Electricity demand forecasting. the focus is on short-term demand forecasting at some aggregate level (e.g., zone or nationwide demands) from data with at least hourly sampled data. The main salient features of the load curve are first highlighted. Some of the common covariates used in the prediction task are also discussed. Then, some basic or now classical methodological approaches for electricity demand forecasting are detailed.

SEQUEL Project-Team

7. New Results

7.1. Decision-making Under Uncertainty

7.1.1. Reinforcement Learning

A Fitted-Q Algorithm for Budgeted MDPs, [26]

We address the problem of budgeted reinforcement learning, in continuous state-space, using a batch of transitions. To this extend, we introduce a novel algorithm called Budgeted Fitted-Q (BFTQ). Benchmarks show that BFTQ performs as well as a regular Fitted-Q algorithm in a continuous 2-D world but also allows one to choose the right amount of budget that fits to a given task without the need of engineering the rewards. We believe that the general principles used to design BFTQ can be applied to extend others classical reinforcement learning algorithms for budgeted oriented applications.

Safe transfer learning for dialogue applications, [27]

In this paper, we formulate the hypothesis that the first dialogues with a new user should be handle in a very conservative way, for two reasons : avoid user dropout; gather more successful dialogues to speedup the learning of the asymptotic strategy. To this extend, we propose to transfer a safe strategy to initiate the first dialogues.

Variance-Aware Regret Bounds for Undiscounted Reinforcement Learning in MDPs, [17]

The problem of reinforcement learning in an unknown and discrete Markov Decision Process (MDP) under the average-reward criterion is considered, when the learner interacts with the system in a single stream of observations, starting from an initial state without any reset. We revisit the minimax lower bound for that problem by making appear the local variance of the bias function in place of the diameter of the MDP. Furthermore, we provide a novel analysis of the KL-Ucrl algorithm establishing a high-probability regret bound scaling as O S s,a V s,a T for this algorithm for ergodic MDPs, where S denotes the number of states and where V s,a is the variance of the bias function with respect to the next-state distribution following action a in state s. The resulting bound improves upon the best previously known regret bound O(DS $\sqrt{}$ AT) for that algorithm, where A and D respectively denote the maximum number of actions (per state) and the diameter of MDP. We finally compare the leading terms of the two bounds in some benchmark MDPs indicating that the derived bound can provide an order of magnitude improvement in some cases. Our analysis leverages novel variations of the transportation lemma combined with Kullback-Leibler concentration inequalities, that we believe to be of independent interest.

Efficient Bias-Span-Constrained Exploration-Exploitation in Reinforcement Learning, [29]

We introduce SCAL, an algorithm designed to perform efficient exploration-exploitation in any unknown weakly-communicating Markov decision process (MDP) for which an upper bound c on the span of the optimal bias function is known. For an MDP with S states, A actions and $\Gamma \leq S$ possible next states, we prove a regret bound of $\widetilde{O}(c\sqrt{\Gamma SAT})$, which significantly improves over existing algorithms (e.g., UCRL and PSRL), whose regret scales linearly with the MDP diameter D. In fact, the optimal bias span is finite and often much smaller than D (e.g., $D = \infty$ in non-communicating MDPs). A similar result was originally derived by Bartlett and Tewari (2009) for REGAL.C, for which no tractable algorithm is available. In this paper, we relax the optimization problem at the core of REGAL.C, we carefully analyze its properties, and we provide the first computationally efficient algorithm to solve it. Finally, we report numerical simulations supporting our theoretical findings and showing how SCAL significantly outperforms UCRL in MDPs with large diameter and small span.

Near Optimal Exploration-Exploitation in Non-Communicating Markov Decision Processes, [28]

While designing the state space of an MDP, it is common to include states that are transient or not reachable by any policy (e.g., in mountain car, the product space of speed and position contains configurations that are not physically reachable). This leads to defining weakly-communicating or multi-chain MDPs. In this paper, we introduce TUCRL, the first algorithm able to perform efficient exploration-exploitation in any finite Markov Decision Process (MDP) without requiring any form of prior knowledge. In particular, for any MDP with S^{C} communicating states, A actions and $\Gamma^{\mathsf{C}} \leq S^{\mathsf{C}}$ possible communicating next states, we derive a $\widetilde{O}(D^{\mathsf{C}}\sqrt{\Gamma^{\mathsf{C}} S^{\mathsf{C}} AT})$ regret bound, where D^{C} is the diameter (i.e., the longest shortest path) of the communicating part of the MDP. This is in contrast with optimistic algorithms (e.g., UCRL, Optimistic PSRL) that suffer linear regret in weakly-communicating MDPs, as well as posterior sampling or regularized algorithms (e.g., REGAL), which require prior knowledge on the bias span of the optimal policy to bias the exploration to achieve sub-linear regret. We also prove that in weakly-communicating MDPs, no algorithm can ever achieve a logarithmic growth of the regret without first suffering a linear regret for a number of steps that is exponential in the parameters of the MDP. Finally, we report numerical simulations supporting our theoretical findings and showing how TUCRL overcomes the limitations of the state-of-the-art.

Upper Confidence Reinforcement Learning exploiting state-action equivalence, [53]

Stochastic Variance-Reduced Policy Gradient, [34]

In this paper, we propose a novel reinforcement-learning algorithm consisting in a stochastic variance-reduced version of policy gradient for solving Markov Decision Processes (MDPs). Stochastic variance-reduced gradient (SVRG) methods have proven to be very successful in supervised learning. However, their adaptation to policy gradient is not straightforward and needs to account for I) a non-concave objective function; II) approximations in the full gradient computation; and III) a non-stationary sampling process. The result is SVRPG, a stochastic variance-reduced policy gradient algorithm that leverages on importance weights to preserve the unbiasedness of the gradient estimate. Under standard assumptions on the MDP, we provide convergence guarantees for SVRPG with a convergence rate that is linear under increasing batch sizes. Finally, we suggest practical variants of SVRPG, and we empirically evaluate them on continuous MDPs.

Importance Weighted Transfer of Samples in Reinforcement Learning, [38]

We consider the transfer of experience samples (i.e., tuples < s, a, s', r >) in reinforcement learning (RL), collected from a set of source tasks to improve the learning process in a given target task. Most of the related approaches focus on selecting the most relevant source samples for solving the target task, but then all the transferred samples are used without considering anymore the discrepancies between the task models. In this paper, we propose a model-based technique that automatically estimates the relevance (importance weight) of each source sample for solving the target task. In the proposed approach, all the samples are transferred and used by a batch RL algorithm to solve the target task, but their contribution to the learning process is proportional to their importance weight. By extending the results for importance weighting provided in supervised learning literature, we develop a finite-sample analysis of the proposed batch RL algorithm. Furthermore, we empirically compare the proposed algorithm to state-of-the-art approaches, showing that it achieves better learning performance and is very robust to negative transfer, even when some source tasks are significantly different from the target task.

Training Dialogue Systems With Human Advice, [20]

One major drawback of Reinforcement Learning (RL) Spoken Dialogue Systems is that they inherit from the general exploration requirements of RL which makes them hard to deploy from an industry perspective. On the other hand, industrial systems rely on human expertise and hand written rules so as to avoid irrelevant behavior to happen and maintain acceptable experience from the user point of view. In this paper, we attempt to bridge the gap between those two worlds by providing an easy way to incorporate all kinds of human expertise in the training phase of a Reinforcement Learning Dialogue System. Our approach, based on the TAMER framework, enables safe and efficient policy learning by combining the traditional Reinforcement Learning reward signal with an additional reward, encoding expert advice. Experimental results show that our method leads to substantial improvements over more traditional Reinforcement Learning methods.

7.1.1.1. Deep reinforcement learning

FiLM: Visual Reasoning with a General Conditioning Layer, [35]

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.

Feature-wise transformations, [13]

Deep Reinforcement Learning and the Deadly Triad, [55]

We know from reinforcement learning theory that temporal difference learning can fail in certain cases. Sutton and Barto (2018) identify a deadly triad of function approximation, bootstrapping, and off-policy learning. When these three properties are combined, learning can diverge with the value estimates becoming unbounded. However, several algorithms successfully combine these three properties, which indicates that there is at least a partial gap in our understanding. In this work, we investigate the impact of the deadly triad in practice, in the context of a family of popular deep reinforcement learning models - deep Q-networks trained with experience replay - analyzing how the components of this system play a role in the emergence of the deadly triad, and in the agent's performance

7.1.2. Multi-armed Bandit Theory

Corrupt Bandits for Preserving Local Privacy, [30]

We study a variant of the stochastic multi-armed bandit (MAB) problem in which the rewards are corrupted. In this framework, motivated by privacy preservation in online recommender systems, the goal is to maximize the sum of the (unobserved) rewards, based on the observation of transformation of these rewards through a stochastic corruption process with known parameters. We provide a lower bound on the expected regret of any bandit algorithm in this corrupted setting. We devise a frequentist algorithm, KLUCB-CF, and a Bayesian algorithm, TS-CF and give upper bounds on their regret. We also provide the appropriate corruption parameters to guarantee a desired level of local privacy and analyze how this impacts the regret. Finally, we present some experimental results that confirm our analysis.

A simple parameter-free and adaptive approach to optimization under a minimal local smoothness assumption, [21]

We study the problem of optimizing a function under a budgeted number of evaluations. We only assume that the function is locally smooth around one of its global optima. The difficulty of optimization is measured in terms of 1) the amount of noise b of the function evaluation and 2) the local smoothness, d, of the function. A smaller d results in smaller optimization error. We come with a new, simple, and parameter-free approach. First, for all values of b and d, this approach recovers at least the state-of-the-art regret guarantees. Second, our approach additionally obtains these results while being agnostic to the values of both b and d. This leads to the first algorithm that naturally adapts to an unknown range of noise b and leads to significant improvements in a moderate and low-noise regime. Third, our approach also obtains a remarkable improvement over the state-of-the-art SOO algorithm when the noise is very low which includes the case of optimization under deterministic feedback ($b = 0$). There, under our minimal local smoothness assumption, this improvement is of exponential magnitude and holds for a class of functions that covers the vast majority of functions that practitioners optimize ($d = 0$). We show that our algorithmic improvement is also borne out in the numerical experiments, where we empirically show faster convergence on common benchmark functions.

Best of both worlds: Stochastic & adversarial best-arm identification, [18]

We study bandit best-arm identification with arbitrary and potentially adversarial rewards. A simple random uniform learner obtains the optimal rate of error in the adversarial scenario. However, this type of strategy is suboptimal when the rewards are sampled stochastically. Therefore, we ask: Can we design a learner that performs optimally in both the stochastic and adversarial problems while not being aware of the nature of the rewards? First, we show that designing such a learner is impossible in general. In particular, to be robust to adversarial rewards, we can only guarantee optimal rates of error on a subset of the stochastic problems. We give a lower bound that characterizes the optimal rate in stochastic problems if the strategy is constrained to be robust to adversarial rewards. Finally, we design a simple parameter-free algorithm and show that its probability of error matches (up to log factors) the lower bound in stochastic problems, and it is also robust to adversarial ones.

Optimistic optimization of a Brownian, [31]

We address the problem of optimizing a Brownian motion. We consider a (random) realization W of a Brownian motion with input space in $[0, 1]$. Given W, our goal is to return an ϵ-approximation of its maximum using the smallest possible number of function evaluations, the sample complexity of the algorithm. We provide an algorithm with sample complexity of order $\log 2\ (1/\epsilon)$. This improves over previous results of Al-Mharmah and Calvin (1996) and Calvin et al. (2017) which provided only polynomial rates. Our algorithm is adaptive-each query depends on previous values-and is an instance of the optimism-in-the-face-of-uncertainty principle.

Rotting bandits are no harder than stochastic ones, [37]

In bandits, arms' distributions are stationary. This is often violated in practice, where rewards change over time. In applications as recommendation systems, online advertising, and crowdsourcing, the changes may be triggered by the pulls, so that the arms' rewards change as a function of the number of pulls. In this paper, we consider the specific case of non-parametric rotting bandits, where the expected reward of an arm may decrease every time it is pulled. We introduce the filtering on expanding window average (FEWA) algorithm that at each round constructs moving averages of increasing windows to identify arms that are more likely to return high rewards when pulled once more. We prove that, without any knowledge on the decreasing behavior of the arms, FEWA achieves similar anytime problem-dependent, $\widetilde{\mathcal{O}}(\log(KT))$, and problem-independent, $\widetilde{\mathcal{O}}(\sqrt{KT})$, regret bounds of near-optimal stochastic algorithms as UCB1 of Auer et al. (2002a). This result substantially improves the prior result of Levine et al. (2017) which needed knowledge of the horizon and decaying parameters to achieve problem-independent bound of only $\widetilde{\mathcal{O}}(K^{1/3}T^{2/3})$. Finally, we report simulations confirming the theoretical improvements of FEWA.

Adaptive black-box optimization got easier: HCT only needs local smoothness, [41]

Hierarchical bandits is an approach for global optimization of extremely irregular functions. This paper provides new elements regarding POO, an adaptive meta-algorithm that does not require the knowledge of local smoothness of the target function. We first highlight the fact that the subroutine algorithm used in POO should have a small regret under the assumption of local smoothness with respect to the chosen partitioning, which is unknown if it is satisfied by the standard subroutine HOO. In this work, we establish such regret guarantee for HCT, which is another hierarchical optimistic optimization algorithm that needs to know the smoothness. This confirms the validity of POO. We show that POO can be used with HCT as a subroutine with a regret upper bound that matches the one of best-known algorithms using the knowledge of smoothness up to a $\sqrt{}$ log n factor.

Boundary Crossing Probabilities for General Exponential Families, [16]

Multi-Player Bandits Revisited, [22]

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 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.

Pure Exploration in Infinitely-Armed Bandit Models with Fixed-Confidence, [19]

We consider the problem of near-optimal arm identification in the fixed confidence setting of the infinitely armed bandit problem when nothing is known about the arm reservoir distribution. We (1) introduce a PAC-like framework within which to derive and cast results; (2) derive a sample complexity lower bound for near-optimal arm identification; (3) propose an algorithm that identifies a nearly-optimal arm with high probability and derive an upper bound on its sample complexity which is within a log factor of our lower bound; and (4) discuss whether our $\log^2(1/\delta)$ dependence is inescapable for "two-phase" (select arms first, identify the best later) algorithms in the infinite setting. This work permits the application of bandit models to a broader class of problems where fewer assumptions hold.

Aggregation of Multi-Armed Bandits Learning Algorithms for Opportunistic Spectrum Access, [23]

Multi-armed bandit algorithms have been recently studied and evaluated for Cognitive Radio (CR), especially in the context of Opportunistic Spectrum Access (OSA). Several solutions have been explored based on various models, but it is hard to exactly predict which could be the best for real-world conditions at every instants. Hence, expert aggregation algorithms can be useful to select on the run the best algorithm for a specific situation. Aggregation algorithms, such as Exp4 dating back from 2002, have never been used for OSA learning, and we show that it appears empirically sub-efficient when applied to simple stochastic problems. In this article, we present an improved variant, called Aggregator. For synthetic OSA problems modeled as Multi-Armed Bandit (MAB) problems, simulation results are presented to demonstrate its empirical efficiency. We combine classical algorithms, such as Thompson sampling, Upper-Confidence Bounds algorithms (UCB and variants), and Bayesian or Kullback-Leibler UCB. Our algorithm offers good performance compared to state-of-the-art algorithms (Exp4, CORRAL or LearnExp), and appears as a robust approach to select on the run the best algorithm for any stochastic MAB problem, being more realistic to real-world radio settings than any tuning-based approach.

What Doubling Tricks Can and Can't Do for Multi-Armed Bandits, [47]

An online reinforcement learning algorithm is anytime if it does not need to know in advance the horizon T of the experiment. A well-known technique to obtain an anytime algorithm from any non-anytime algorithm is the "Doubling Trick". In the context of adversarial or stochastic multi-armed bandits, the performance of an algorithm is measured by its regret, and we study two families of sequences of growing horizons (geometric and exponential) to generalize previously known results that certain doubling tricks can be used to conserve certain regret bounds. In a broad setting, we prove that a geometric doubling trick can be used to conserve (minimax) bounds in $R\_T = O(\sqrt{T})$ but cannot conserve (distribution-dependent) bounds in $R\_T = O(\log T)$. We give insights as to why exponential doubling tricks may be better, as they conserve bounds in $R\_T = O(\log T)$, and are close to conserving bounds in $R\_T = O(\sqrt{T})$.

Mixture Martingales Revisited with Applications to Sequential Tests and Confidence Intervals, [50]

This paper presents new deviation inequalities that are valid uniformly in time under adaptive sampling in a multi-armed bandit model. The deviations are measured using the Kullback-Leibler divergence in a given one-dimensional exponential family, and may take into account several arms at a time. They are obtained by constructing for each arm a mixture martingale based on a hierarchical prior, and by multiplying those martingales. Our deviation inequalities allow us to analyze stopping rules based on generalized likelihood ratios for a large class of sequential identification problems, and to construct tight confidence intervals for some functions of the means of the arms.

7.1.3. Stochastic Games

Actor-Critic Fictitious Play in Simultaneous Move Multistage Games, [36]

Fictitious play is a game theoretic iterative procedure meant to learn an equilibrium in normal form games. However, this algorithm requires that each player has full knowledge of other players' strategies. Using an architecture inspired by actor-critic algorithms, we build a stochastic approximation of the fictitious play process. This procedure is on-line, decentralized (an agent has no information of others' strategies and rewards) and applies to multistage games (a generalization of normal form games). In addition, we prove convergence of our method towards a Nash equilibrium in both the cases of zero-sum two-player multistage games and cooperative multistage games. We also provide empirical evidence of the soundness of our approach on the game of Alesia with and without function approximation.

Sequential Test for the Lowest Mean: From Thompson to Murphy Sampling, [39]

Learning the minimum/maximum mean among a finite set of distributions is a fundamental sub-task in planning, game tree search and reinforcement learning. We formalize this learning task as the problem of sequentially testing how the minimum mean among a finite set of distributions compares to a given threshold. We develop refined non-asymptotic lower bounds, which show that optimality mandates very different sampling behavior for a low vs high true minimum. We show that Thompson Sampling and the intuitive Lower Confidence Bounds policy each nail only one of these cases. We develop a novel approach that we call Murphy Sampling. Even though it entertains exclusively low true minima, we prove that MS is optimal for both possibilities. We then design advanced self-normalized deviation inequalities, fueling more aggressive stopping rules. We complement our theoretical guarantees by experiments showing that MS works best in practice.

7.1.4. Online Kernel and Graph-Based Methods

Improved large-scale graph learning through ridge spectral sparsification, [25]

The representation and learning benefits of methods based on graph Laplacians, such as Laplacian smoothing or harmonic function solution for semi-supervised learning (SSL), are empirically and theoretically well supported. Nonetheless , the exact versions of these methods scale poorly with the number of nodes n of the graph. In this paper, we combine a spectral sparsification routine with Laplacian learning. Given a graph G as input, our algorithm computes a sparsifier in a distributed way in $O(n \log 3(n))$ time, $O(m \log 3(n))$ work and $O(n \log(n))$ memory, using only $\log(n)$ rounds of communication. Furthermore , motivated by the regularization often employed in learning algorithms, we show that constructing sparsifiers that preserve the spectrum of the Laplacian only up to the regularization level may drastically reduce the size of the final graph. By constructing a spectrally-similar graph, we are able to bound the error induced by the sparsification for a variety of downstream tasks (e.g., SSL). We empirically validate the theoretical guarantees on Amazon co-purchase graph and compare to the state-of-the-art heuristics.

DPPy: Sampling Determinantal Point Processes with Python, [49]

Determinantal point processes (DPPs) are specific probability distributions over clouds of points that are used as models and computational tools across physics, probability, statistics, and more recently machine learning. Sampling from DPPs is a challenge and therefore we present DPPy, a Python toolbox that gathers known exact and approximate sampling algorithms. The project is hosted on GitHub and equipped with an extensive documentation. This documentation takes the form of a short survey of DPPs and relates each mathematical property with DPPy objects.

Streaming kernel regression with provably adaptive mean, variance, and regularization, [14]

We consider the problem of streaming kernel regression, when the observations arrive sequentially and the goal is to recover the underlying mean function, assumed to belong to an RKHS. The variance of the noise is not assumed to be known. In this context, we tackle the problem of tuning the regularization parameter adaptively at each time step, while maintaining tight confidence bounds estimates on the value of the mean function at each point. To this end, we first generalize existing results for finite-dimensional linear regression with fixed regularization and known variance to the kernel setup with a regularization parameter allowed to be a measurable function of past observations. Then, using appropriate self-normalized inequalities we build upper and lower bound estimates for the variance, leading to Bersntein-like concentration bounds. The later is used in

order to define the adaptive regularization. The bounds resulting from our technique are valid uniformly over all observation points and all time steps, and are compared against the literature with numerical experiments. Finally, the potential of these tools is illustrated by an application to kernelized bandits, where we revisit the Kernel UCB and Kernel Thompson Sampling procedures, and show the benefits of the novel adaptive kernel tuning strategy.

7.2. Applications

7.2.1. Dialogue Systems and Natural Language

FiLM: Visual Reasoning with a General Conditioning Layer, [35]

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.

End-to-End Automatic Speech Translation of Audiobooks, [24]

We investigate end-to-end speech-to-text translation on a corpus of audiobooks specifically augmented for this task. Previous works investigated the extreme case where source language transcription is not available during learning nor decoding , but we also study a midway case where source language transcription is available at training time only. In this case, a single model is trained to decode source speech into target text in a single pass. Experimental results show that it is possible to train compact and efficient end-to-end speech translation models in this setup. We also distribute the corpus and hope that our speech translation baseline on this corpus will be challenged in the future.

Visual Reasoning with Multi-hop Feature Modulation, [42]

Recent breakthroughs in computer vision and natural language processing have spurred interest in challenging multi-modal tasks such as visual question-answering and visual dialogue. For such tasks, one successful approach is to condition image-based convolutional network computation on language via Feature-wise Linear Modulation (FiLM) layers, i.e., per-channel scaling and shifting. We propose to generate the parameters of FiLM layers going up the hierarchy of a convolutional network in a multi-hop fashion rather than all at once, as in prior work. By alternating between attending to the language input and generating FiLM layer parameters, this approach is better able to scale to settings with longer input sequences such as dialogue. We demonstrate that multi-hop FiLM generation achieves state-of-the-art for the short input sequence task ReferIt-on-par with single-hop FiLM generation-while also significantly outperforming prior state-of-the-art and single-hop FiLM generation on the GuessWhat?! visual dialogue task.

7.2.2. Recommendation systems

Recurrent Neural Networks for Long and Short-Term Sequential Recommendation, [54]

Recommender systems objectives can be broadly characterized as modeling user preferences over short- or long-term time horizon. A large body of previous research studied long-term recommendation through dimensionality reduction techniques applied to the historical user-item interactions. A recently introduced session-based recommendation setting highlighted the importance of modeling short-term user preferences. In this task, Recurrent Neural Networks (RNN) have shown to be successful at capturing the nuances of user's interactions within a short time window. In this paper, we evaluate RNN-based models on both short-term and long-term recommendation tasks. Our experimental results suggest that RNNs are capable of predicting immediate as well as distant user interactions. We also find the best performing configuration to be a stacked RNN with layer normalization and tied item embeddings.

Fighting Boredom in Recommender Systems with Linear Reinforcement Learning, [43]

A common assumption in recommender systems (RS) is the existence of a best fixed recommendation strategy. Such strategy may be simple and work at the item level (e.g., in multi-armed bandit it is assumed one best fixed arm/item exists) or implement more sophisticated RS (e.g., the objective of A/B testing is to find the best fixed RS and execute it thereafter). We argue that this assumption is rarely verified in practice, as the recommendation process itself may impact the user's preferences. For instance, a user may get bored by a strategy, while she may gain interest again, if enough time passed since the last time that strategy was used. In this case, a better approach consists in alternating different solutions at the right frequency to fully exploit their potential. In this paper, we first cast the problem as a Markov decision process, where the rewards are a linear function of the recent history of actions, and we show that a policy considering the long-term influence of the recommendations may outperform both fixed-action and contextual greedy policies. We then introduce an extension of the UCRL algorithm (LINUCRL) to effectively balance exploration and exploitation in an unknown environment, and we derive a regret bound that is independent of the number of states. Finally, we empirically validate the model assumptions and the algorithm in a number of realistic scenarios.

7.2.3. Autonomous car

A Survey of State-Action Representations for Autonomous Driving, [51]

Approximate Robust Control of Uncertain Dynamical Systems, [40]

This work studies the design of safe control policies for large-scale non-linear systems operating in uncertain environments. In such a case, the robust control framework is a principled approach to safety that aims to maximize the worst-case performance of a system. However, the resulting optimization problem is generally intractable for non-linear systems with continuous states. To overcome this issue, we introduce two tractable methods that are based either on sampling or on a conservative approximation of the robust objective. The proposed approaches are applied to the problem of autonomous driving.

7.2.4. Software development

Correctness Attraction: A Study of Stability of Software Behavior Under Runtime Perturbation, [12]

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.

This paper has attracted a significant interest in the SE community. This work has been invited for an oral presentation (along a 1 page summary) at the 40th International Conference on Software Engineering, the main conference in software engineering. It has then been invited on the IEEE Software review blog.

SMPyBandits: an Experimental Framework for Single and Multi-Players Multi-Arms Bandits Algorithms in Python, [46]

SMPyBandits is a package for numerical simulations on single-player and multi-players Multi-Armed Bandits (MAB) algorithms, written in Python (2 or 3). This library is the most complete open-source implementation of state-of-the-art algorithms tackling various kinds of sequential learning problems referred to as Multi-Armed Bandits. It is extensive, simple to use and maintain, with a clean and well documented codebase. It allows fast prototyping of experiments, with an easy configuration system and command-line options to customize experiments.

Lilian Besson developed a library for multi-armed bandit algorithms in Python for single and multi-player bandits.

7.2.5. Deep Learning

FiLM: Visual Reasoning with a General Conditioning Layer, [35]

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.

Feature-wise transformations, [13]

i-RevNet: Deep Invertible Networks, [32]

It is widely believed that the success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand. This is supported empirically by the difficulty of recovering images from their hidden representations, in most commonly used network architectures. In this paper we show via a one-to-one mapping that this loss of information is not a necessary condition to learn representations that generalize well on complicated problems, such as ImageNet. Via a cascade of homeomorphic layers, we build the i-RevNet, a network that can be fully inverted up to the final projection onto the classes, i.e. no information is discarded. Building an invertible architecture is difficult, for one, because the local inversion is ill-conditioned, we overcome this by providing an explicit inverse. An analysis of i-RevNets learned representations suggests an alternative explanation for the success of deep networks by a progressive contraction and linear separation with depth. To shed light on the nature of the model learned by the i-RevNet we reconstruct linear interpolations between natural image representations.

Compressing the Input for CNNs with the First-Order Scattering Transform, [33]

We study the first-order scattering transform as a candidate for reducing the signal processed by a convolutional neural network (CNN). We study this transformation and show theoretical and empirical evidence that in the case of natural images and sufficiently small translation invariance, this transform preserves most of the signal information needed for classification while substantially reducing the spatial resolution and total signal size. We show that cascading a CNN with this representation performs on par with ImageNet classification models commonly used in downstream tasks such as the ResNet-50. We subsequently apply our trained hybrid ImageNet model as a base model on a detection system, which has typically larger image inputs. On Pascal VOC and COCO detection tasks we deliver substantial improvements in the inference speed and training memory consumption compared to models trained directly on the input image.

Visual Reasoning with Multi-hop Feature Modulation, [42]

Recent breakthroughs in computer vision and natural language processing have spurred interest in challenging multi-modal tasks such as visual question-answering and visual dialogue. For such tasks, one successful approach is to condition image-based convolutional network computation on language via Feature-wise Linear Modulation (FiLM) layers, i.e., per-channel scaling and shifting. We propose to generate the parameters of FiLM layers going up the hierarchy of a convolutional network in a multi-hop fashion rather than all at once, as in prior work. By alternating between attending to the language input and generating FiLM layer parameters, this approach is better able to scale to settings with longer input sequences such as dialogue. We demonstrate that multi-hop FiLM generation achieves state-of-the-art for the short input sequence task ReferIt-on-par with single-hop FiLM generation-while also significantly outperforming prior state-of-the-art and single-hop FiLM generation on the GuessWhat?! visual dialogue task.

SIERRA Project-Team

7. New Results

7.1. On the Global Convergence of Gradient Descent for Over-parameterized Models using Optimal Transport

Many tasks in machine learning and signal processing can be solved by minimizing a convex function of a measure. This includes sparse spikes deconvolution or training a neural network with a single hidden layer. For these problems, in [25] we study a simple minimization method: the unknown measure is discretized into a mixture of particles and a continuous-time gradient descent is performed on their weights and positions. This is an idealization of the usual way to train neural networks with a large hidden layer. We show that, when initialized correctly and in the many-particle limit, this gradient flow, although non-convex, converges to global minimizers. The proof involves Wasserstein gradient flows, a by-product of optimal transport theory. Numerical experiments show that this asymptotic behavior is already at play for a reasonable number of particles, even in high dimension.

7.2. Sharp Analysis of Learning with Discrete Losses

In [49], we study a least-squares framework to systematically design learning algorithms for discrete losses, with quantitative characterizations in terms of statistical and computational complexity. In particular we improve existing results by providing explicit dependence on the number of labels for a wide class of losses and faster learning rates in conditions of low-noise. Theoretical results are complemented with experiments on real datasets, showing the effectiveness of the proposed general approach.

7.3. Gossip of Statistical Observations using Orthogonal Polynomials

Consider a network of agents connected by communication links, where each agent holds a real value. The gossip problem consists in estimating the average of the values diffused in the network in a distributed manner. Current techniques for gossiping are designed to deal with worst-case scenarios, which is irrelevant in applications to distributed statistical learning and denoising in sensor networks. In [39], we design second-order gossip methods tailor-made for the case where the real values are i.i.d. samples from the same distribution. In some regular network structures, we are able to prove optimality of our methods, and simulations suggest that they are efficient in a wide range of random networks. Our approach of gossip stems from a new acceleration framework using the family of orthogonal polynomials with respect to the spectral measure of the network graph.

7.4. Marginal Weighted Maximum Log-likelihood for Efficient Learning of Perturb-and-Map models

In [20], We consider the structured-output prediction problem through probabilistic approaches and generalize the “perturb-and-MAP” framework to more challenging weighted Hamming losses, which are crucial in applications. While in principle our approach is a straightforward marginalization, it requires solving many related MAP inference problems. We show that for log-supermodular pairwise models these operations can be performed efficiently using the machinery of dynamic graph cuts. We also propose to use double stochastic gradient descent, both on the data and on the perturbations, for efficient learning. Our framework can naturally take weak supervision (e.g., partial labels) into account. We conduct a set of experiments on medium-scale character recognition and image segmentation, showing the benefits of our algorithms.

7.5. Slice inverse regression with score functions

In [6], we consider non-linear regression problems where we assume that the response depends non-linearly on a linear projection of the covariates. We propose score function extensions to sliced inverse regression problems, both for the first- order and second-order score functions. We show that they provably improve estimation in the population case over the non-sliced versions and we study finite sample estimators and their consistency given the exact score functions. We also propose to learn the score function as well, in two steps, i.e., first learning the score function and then learning the effective dimension reduction space, or directly, by solving a convex optimization problem regularized by the nuclear norm. We illustrate our results on a series of experiments.

7.6. Constant Step Size Stochastic Gradient Descent for Probabilistic Modeling

Stochastic gradient methods enable learning probabilistic models from large amounts of data. While large step-sizes (learning rates) have shown to be best for least-squares (e.g., Gaussian noise) once combined with parameter averaging, these are not leading to convergent algorithms in general. In this paper, we consider generalized linear models, that is, conditional models based on exponential families. In [14], we propose averaging moment parameters instead of natural parameters for constant-step-size stochastic gradient descent. For finite-dimensional models, we show that this can sometimes (and surprisingly) lead to better predictions than the best linear model. For infinite-dimensional models, we show that it always converges to optimal predictions, while averaging natural parameters never does. We illustrate our findings with simulations on synthetic data and classical benchmarks with many observations.

7.7. Nonlinear Acceleration of Momentum and Primal-Dual Algorithms

In [40], We describe a convergence acceleration scheme for multistep optimization algorithms. The extrapolated solution is written as a nonlinear average of the iterates produced by the original optimization algorithm. Our scheme does not need the underlying fixed-point operator to be symmetric, hence handles e.g. algorithms with momentum terms such as Nesterov's accelerated method, or primal-dual methods. The weights are computed via a simple linear system and we analyze performance in both online and offline modes. We use Crouzeix's conjecture to show that acceleration performance is controlled by the solution of a Chebyshev problem on the numerical range of a non-symmetric operator modelling the behavior of iterates near the optimum. Numerical experiments are detailed on image processing problems, logistic regression and neural network training for CIFAR10 and ImageNet.

7.8. Nonlinear Acceleration of Deep Neural Networks

Regularized nonlinear acceleration (RNA) is a generic extrapolation scheme for optimization methods, with marginal computational overhead. It aims to improve convergence using only the iterates of simple iterative algorithms. However, so far its application to optimization was theoretically limited to gradient descent and other single-step algorithms. Here, we adapt RNA to a much broader setting including stochastic gradient with momentum and Nesterov's fast gradient. In [54], we use it to train deep neural networks, and empirically observe that extrapolated networks are more accurate, especially in the early iterations. A straightforward application of our algorithm when training ResNet-152 on ImageNet produces a top-1 test error of 20.88, improving by 0.8 the reference classification pipeline. Furthermore, the code runs offline in this case, so it never negatively affects performance.

7.9. Nonlinear Acceleration of CNNs

The Regularized Nonlinear Acceleration (RNA) algorithm is an acceleration method capable of improving the rate of convergence of many optimization schemes such as gradient descend, SAGA or SVRG. Until now, its analysis is limited to convex problems, but empirical observations shows that RNA may be extended to wider settings. In [36], we investigate further the benefits of RNA when applied to neural networks, in particular for the task of image recognition on CIFAR10 and ImageNet. With very few modifications of exiting frameworks, RNA improves slightly the optimization process of CNNs, after training.

7.10. Robust Seriation and Applications To Cancer Genomics

The seriation problem seeks to reorder a set of elements given pairwise similarity information, so that elements with higher similarity are closer in the resulting sequence. When a global ordering consistent with the similarity information exists, an exact spectral solution recovers it in the noiseless case and seriation is equivalent to the combinatorial 2-SUM problem over permutations, for which several relaxations have been derived. However, in applications such as DNA assembly, similarity values are often heavily corrupted, and the solution of 2-SUM may no longer yield an approximate serial structure on the elements. In [52], we introduce the robust seriation problem and show that it is equivalent to a modified 2-SUM problem for a class of similarity matrices modeling those observed in DNA assembly. We explore several relaxations of this modified 2-SUM problem and compare them empirically on both synthetic matrices and real DNA data. We then introduce the problem of seriation with duplications, which is a generalization of Seriation motivated by applications to cancer genome reconstruction. We propose an algorithm involving robust seriation to solve it, and present preliminary results on synthetic data sets.

7.11. Reconstructing Latent Orderings by Spectral Clustering

Spectral clustering uses a graph Laplacian spectral embedding to enhance the cluster structure of some data sets. When the embedding is one dimensional, it can be used to sort the items (spectral ordering). A number of empirical results also suggests that a multidimensional Laplacian embedding enhances the latent ordering of the data, if any. This also extends to circular orderings, a case where unidimensional embeddings fail. In [51], we tackle the task of retrieving linear and circular orderings in a unifying framework, and show how a latent ordering on the data translates into a filamentary structure on the Laplacian embedding. We propose a method to recover it, illustrated with numerical experiments on synthetic data and real DNA sequencing data.

7.12. Lyapunov Functions for First-Order Methods: Tight Automated Convergence Guarantees

In [21], we present a novel way of generating Lyapunov functions for proving linear convergence rates of first-order optimization methods. Our approach provably obtains the fastest linear convergence rate that can be verified by a quadratic Lyapunov function (with given states), and only relies on solving a small-sized semidefinite program. Our approach combines the advantages of performance estimation problems and integral quadratic constraints, and relies on convex interpolation.

7.13. Efficient First-order Methods for Convex Minimization: a Constructive Approach

In [44], we describe a novel constructive technique for devising efficient first-order methods for a wide range of large-scale convex minimization settings, including smooth, non-smooth, and strongly convex minimization. The design technique takes a method performing a series of subspace-searches and constructs a family of methods that share the same worst-case guarantees as the original method, and includes a fixed-step first-order method. We show that this technique yields optimal methods in the smooth and non-smooth cases and derive new methods for these cases, including methods that forego knowledge of the problem parameters, at the cost of a one-dimensional line search per iteration. In the strongly convex case, we show how numerical tools can be used to perform the construction, and show that resulting method offers an improved convergence rate compared to Nesterov's celebrated fast gradient method.

7.14. Operator Splitting Performance Estimation: Tight contraction factors and optimal parameter selection

In [53], we propose a methodology for studying the performance of common splitting methods through semidefinite programming. We prove tightness of the methodology and demonstrate its value by presenting

two applications of it. First, we use the methodology as a tool for computer-assisted proofs to prove tight analytical contraction factors for Douglas–Rachford splitting that are likely too complicated for a human to find bare-handed. Second, we use the methodology as an algorithmic tool to computationally select the optimal splitting method parameters by solving a series of semidefinite programs.

7.15. Finite-sample Analysis of M-estimators using Self-concordance

In [50], we demonstrate how *self-concordance* of the loss allows to obtain asymptotically optimal rates for M-estimators in finite-sample regimes. We consider two classes of losses: (i) self-concordant losses, i.e., whose third derivative is uniformly bounded with the $3/2$ power of the second; (ii) *pseudo* self-concordant losses, for which the power is removed. These classes contain some losses arising in generalized linear models, including the logistic loss; in addition, the second class includes some common pseudo-Huber losses. Our results consist in establishing the *critical sample size* sufficient to reach the asymptotically optimal excess risk in both cases. Denoting d the parameter dimension, and d_e the effective dimension taking into account possible model misspecification, we find the critical sample size to be $O(d_e \cdot d)$ for the first class of losses, and $O(\rho \cdot d_e \cdot d)$ for the second class, where ρ is the problem-dependent parameter that characterizes the risk curvature at the best predictor θ_*. In contrast to the existing results, we only impose *local* assumptions on the data distribution, assuming that the calibrated design, i.e., the design scaled with the square root of the second derivative of the loss, is subgaussian at the best predictor. Moreover, we obtain the improved bounds on the critical sample size, scaling *near-linearly* in $\max(d_e, d)$, under the extra assumption that the calibrated design is subgaussian in the Dikin ellipsoid of θ_*. Motivated by these findings, we construct canonically self-concordant analogues of the Huber and logistic losses with improved statistical properties. Finally, we extend some of the above results to ℓ_1-penalized M-estimators in high-dimensional setups.

7.16. Uniform regret bounds over R^d for the sequential linear regression problem with the square loss

In [45] we consider the setting of online linear regression for arbitrary deterministic sequences, with the square loss. We are interested in obtaining regret bounds that hold uniformly over all vectors R^d. When the feature sequence is known at the beginning of the game, they provided closed-form regret bounds of $2dB^2 \ln T + O(1)$, where T is the number of rounds and B is a bound on the observations. Instead, we derive bounds with an optimal constant of 1 in front of the $dB^2 \ln T$ term. In the case of sequentially revealed features, we also derive an asymptotic regret bound of $dB^2 \ln T$ for any individual sequence of features and bounded observations. All our algorithms are variants of the online nonlinear ridge regression forecaster, either with a data-dependent regularization or with almost no regularization.

7.17. Efficient online algorithms for fast-rate regret bounds under sparsity.

In [46] we consider the problem of online convex optimization in two different settings: arbitrary and i.i.d. sequence of convex loss functions. In both settings, we provide efficient algorithms whose cumulative excess risks are controlled with fast-rate sparse bounds. First, the excess risks bounds depend on the sparsity of the objective rather than on the dimension of the parameters space. Second, their rates are faster than the slow-rate $1/\sqrt{T}$

7.18. Exponential convergence of testing error for stochastic gradient methods

In [32], 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.

7.19. Statistical Optimality of Stochastic Gradient Descent on Hard Learning Problems through Multiple Passes

In [33], we consider stochastic gradient descent (SGD) for least-squares regression with potentially several passes over the data. While several passes have been widely reported to perform practically better in terms of predictive performance on unseen data, the existing theoretical analysis of SGD suggests that a single pass is statistically optimal. While this is true for low-dimensional easy problems, we show that for hard problems, multiple passes lead to statistically optimal predictions while single pass does not; we also show that in these hard models, the optimal number of passes over the data increases with sample size. In order to define the notion of hardness and show that our predictive performances are optimal, we consider potentially infinite-dimensional models and notions typically associated to kernel methods, namely, the decay of eigenvalues of the covariance matrix of the features and the complexity of the optimal predictor as measured through the covariance matrix. We illustrate our results on synthetic experiments with non-linear kernel methods and on a classical benchmark with a linear model.

7.20. Central Limit Theorem for stationary Fleming–Viot particle systems in finite spaces

In [11], we consider the Fleming–Viot particle system associated with a continuous-time Markov chain in a finite space. Assuming irreducibility, it is known that the particle system possesses a unique stationary distribution, under which its empirical measure converges to the quasistationary distribution of the Markov chain. We complement this Law of Large Numbers with a Central Limit Theorem. Our proof essentially relies on elementary computations on the infinitesimal generator of the Fleming–Viot particle system, and involves the so-called π-return process in the expression of the asymptotic variance. Our work can be seen as an infinite-time version, in the setting of finite space Markov chains, of results by Del Moral and Miclo [ESAIM: Probab. Statist., 2003] and Cérou, Delyon, Guyader and Rousset [arXiv:1611.00515, arXiv:1709.06771].

7.21. SeaRNN: Improved RNN training through Global-Local Losses

In [16], we propose SEARNN, a novel training algorithm for recurrent neural networks (RNNs) inspired by the "learning to search" (L2S) approach to structured prediction. RNNs have been widely successful in structured prediction applications such as machine translation or parsing, and are commonly trained using maximum likelihood estimation (MLE). Unfortunately, this training loss is not always an appropriate surrogate for the test error: by only maximizing the ground truth probability, it fails to exploit the wealth of information offered by structured losses. Further, it introduces discrepancies between training and predicting (such as exposure bias) that may hurt test performance. Instead, SEARNN leverages test-alike search space exploration to introduce global-local losses that are closer to the test error. We first demonstrate improved performance over MLE on two different tasks: OCR and spelling correction. Then, we propose a subsampling strategy to enable SEARNN to scale to large vocabulary sizes. This allows us to validate the benefits of our approach on a machine translation task.

7.22. Improved asynchronous parallel optimization analysis for stochastic incremental methods

As datasets continue to increase in size and multi-core computer architectures are developed, asynchronous parallel optimization algorithms become more and more essential to the field of Machine Learning. Unfortunately, conducting the theoretical analysis of asynchronous methods is difficult, notably due to the introduction of delay and inconsistency in inherently sequential algorithms. Handling these issues often requires resorting to simplifying but unrealistic assumptions. Through a novel perspective, in [10] we revisit and clarify 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 introduced "perturbed iterate" framework that resolves it. We demonstrate the usefulness of our new framework by analyzing three distinct

asynchronous parallel incremental optimization algorithms: Hogwild (asynchronous SGD), KROMAGNON (asynchronous SVRG) and ASAGA, a novel asynchronous parallel version of the incremental gradient algorithm SAGA that enjoys fast linear convergence rates. We are able to both remove problematic assumptions and obtain better theoretical results. Notably, we prove that ASAGA and KROMAGNON 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 speedups as well as the hardware overhead. Finally, we investigate the overlap constant, an ill-understood but central quantity for the theoretical analysis of asynchronous parallel algorithms. We find that it encompasses much more complexity than suggested in previous work, and often is order-of-magnitude bigger than traditionally thought.

7.23. Asynchronous optimisation for Machine Learning

The impressive breakthroughs of the last two decades in the field of machine learning can be in large part attributed to the explosion of computing power and available data. These two limiting factors have been replaced by a new bottleneck: algorithms. The focus of this thesis [3] is thus on introducing novel methods that can take advantage of high data quantity and computing power. We present two independent contributions.

First, we develop and analyze novel fast optimization algorithms which take advantage of the advances in parallel computing architecture and can handle vast amounts of data. We introduce a new framework of analysis for asynchronous parallel incremental algorithms, which enable correct and simple proofs. We then demonstrate its usefulness by performing the convergence analysis for several methods, including two novel algorithms.

Asaga is a sparse asynchronous parallel variant of the variance-reduced algorithm Saga which enjoys fast linear convergence rates on smooth and strongly convex objectives. We prove that it can be linearly faster than its sequential counterpart, even without sparsity assump- tions.

ProxAsaga is an extension of Asaga to the more general setting where the regularizer can be non-smooth. We prove that it can also achieve a linear speedup. We provide extensive experiments comparing our new algorithms to the current state-of-art.

Second, we introduce new methods for complex struc- tured prediction tasks. We focus on recurrent neural net- works (RNNs), whose traditional training algorithm for RNNs – based on maximum likelihood estimation (MLE) – suffers from several issues. The associated surrogate training loss notably ignores the information contained in structured losses and introduces discrepancies between train and test times that may hurt performance.

To alleviate these problems, we propose SeaRNN, a novel training algorithm for RNNs inspired by the "learning to search" approach to structured prediction.SeaRNN leverages test-alike search space exploration to introduce global-local losses that are closer to the test error than the MLE objective.

We demonstrate improved performance over MLE on three challenging tasks, and provide several subsampling strategies to enable SeaRNN to scale to large-scale tasks, such as machine translation. Finally, after contrasting the behavior of SeaRNN models to MLE models, we conduct an in-depth comparison of our new approach to the related work.

7.24. M^*-Regularized Dictionary Learning

In [38], we derive a performance measure for dictionaries in compressed sensing, based on the M^* of the corresponding norm. We use this measure to regularize dictionary learning algorithms and study the performance of our methods on both compression and inpainting experiments.

7.25. Optimal Algorithms for Non-Smooth Distributed Optimization in Networks

In [35], we consider the distributed optimization of non-smooth convex functions using a network of computing units. We investigate this problem under two regularity assumptions: (1) the Lipschitz continuity

of the global objective function, and (2) the Lipschitz continuity of local individual functions. Under the local regularity assumption, we provide the first optimal first-order decentralized algorithm called multi-step primal-dual (MSPD) and its corresponding optimal convergence rate. A notable aspect of this result is that, for non-smooth functions, while the dominant term of the error is in $O(1/\sqrt{t})$, the structure of the communication network only impacts a second-order term in $O(1/t)$, where t is time. In other words, the error due to limits in communication resources decreases at a fast rate even in the case of non-strongly-convex objective functions. Under the global regularity assumption, we provide a simple yet efficient algorithm called distributed randomized smoothing (DRS) based on a local smoothing of the objective function, and show that DRS is within a $d^{1/4}$ multiplicative factor of the optimal convergence rate, where d is the underlying dimension.

7.26. Relating Leverage Scores and Density using Regularized Christoffel Functions

Statistical leverage scores emerged as a fundamental tool for matrix sketching and column sampling with applications to low rank approximation, regression, random feature learning and quadrature. Yet, the very nature of this quantity is barely understood. Borrowing ideas from the orthogonal polynomial literature, we introduce in [31] the regularized Christoffel function associated to a positive definite kernel. This uncovers a variational formulation for leverage scores for kernel methods and allows to elucidate their relationships with the chosen kernel as well as population density. Our main result quantitatively describes a decreasing relation between leverage score and population density for a broad class of kernels on Euclidean spaces. Numerical simulations support our findings.

7.27. Averaging Stochastic Gradient Descent on Riemannian Manifolds

In [37] we consider the minimization of a function defined on a Riemannian manifold M accessible only through unbiased estimates of its gradients. We develop a geometric framework to transform a sequence of slowly converging iterates generated from stochastic gradient descent (SGD) on M to an averaged iterate sequence with a robust and fast $O(1/n)$ convergence rate. We then present an application of our framework to geodesically-strongly-convex (and possibly Euclidean non-convex) problems. Finally, we demonstrate how these ideas apply to the case of streaming k-PCA, where we show how to accelerate the slow rate of the randomized power method (without requiring knowledge of the eigengap) into a robust algorithm achieving the optimal rate of convergence.

7.28. Localized Structured Prediction

Key to structured prediction is exploiting the problem structure to simplify the learning process. A major challenge arises when data exhibit a local structure (e.g., are made by "parts") that can be leveraged to better approximate the relation between (parts of) the input and (parts of) the output. Recent literature on signal processing, and in particular computer vision, has shown that capturing these aspects is indeed essential to achieve state-of-the-art performance. While such algorithms are typically derived on a case-by-case basis, in [42] we propose the first theoretical framework to deal with part-based data from a general perspective. We derive a novel approach to deal with these problems and study its generalization properties within the setting of statistical learning theory. Our analysis is novel in that it explicitly quantifies the benefits of leveraging the part-based structure of the problem with respect to the learning rates of the proposed estimator.

7.29. Optimal rates for spectral algorithms with least-squares regression over Hilbert spaces

In [12], we study regression problems over a separable Hilbert space with the square loss, covering non-parametric regression over a reproducing kernel Hilbert space. We investigate a class of spectral-regularized algorithms, including ridge regression, principal component analysis, and gradient methods. We prove optimal,

high-probability convergence results in terms of variants of norms for the studied algorithms, considering a capacity assumption on the hypothesis space and a general source condition on the target function. Consequently, we obtain almost sure convergence results with optimal rates. Our results improve and generalize previous results, filling a theoretical gap for the non-attainable cases.

7.30. Differential Properties of Sinkhorn Approximation for Learning with Wasserstein Distance

Applications of optimal transport have recently gained remarkable attention thanks to the computational advantages of entropic regularization. However, in most situations the Sinkhorn approximation of the Wasserstein distance is replaced by a regularized version that is less accurate but easy to differentiate. In [17] we characterize the differential properties of the original Sinkhorn distance, proving that it enjoys the same smoothness as its regularized version and we explicitly provide an efficient algorithm to compute its gradient. We show that this result benefits both theory and applications: on one hand, high order smoothness confers statistical guarantees to learning with Wasserstein approximations. On the other hand, the gradient formula allows us to efficiently solve learning and optimization problems in practice. Promising preliminary experiments complement our analysis.

7.31. Learning with SGD and Random Features

Sketching and stochastic gradient methods are arguably the most common techniques to derive efficient large scale learning algorithms. In [15], we investigate their application in the context of nonparametric statistical learning. More precisely, we study the estimator defined by stochastic gradient with mini batches and random features. The latter can be seen as form of nonlinear sketching and used to define approximate kernel methods. The considered estimator is not explicitly penalized/constrained and regularization is implicit. Indeed, our study highlights how different parameters, such as number of features, iterations, step-size and mini-batch size control the learning properties of the solutions. We do this by deriving optimal finite sample bounds, under standard assumptions. The obtained results are corroborated and illustrated by numerical experiments.

7.32. Manifold Structured Prediction

Structured prediction provides a general framework to deal with supervised problems where the outputs have semantically rich structure. While classical approaches consider finite, albeit potentially huge, output spaces, in [19] we discuss how structured prediction can be extended to a continuous scenario. Specifically, we study a structured prediction approach to manifold valued regression. We characterize a class of problems for which the considered approach is statistically consistent and study how geometric optimization can be used to compute the corresponding estimator. Promising experimental results on both simulated and real data complete our study.

7.33. On Fast Leverage Score Sampling and Optimal Learning

Leverage score sampling provides an appealing way to perform approximate computations for large matrices. Indeed, it allows to derive faithful approximations with a complexity adapted to the problem at hand. Yet, performing leverage scores sampling is a challenge in its own right requiring further approximations. In [18], we study the problem of leverage score sampling for positive definite matrices defined by a kernel. Our contribution is twofold. First we provide a novel algorithm for leverage score sampling and second, we exploit the proposed method in statistical learning by deriving a novel solver for kernel ridge regression. Our main technical contribution is showing that the proposed algorithms are currently the most efficient and accurate for these problems.

7.34. Accelerated Decentralized Optimization with Local Updates for Smooth and Strongly Convex Objectives

In [47], we study the problem of minimizing a sum of smooth and strongly convex functions split over the nodes of a network in a decentralized fashion. We propose a decentralized accelerated algorithm that only requires local synchrony. Its rate depends on the condition number κ of the local functions as well as the network topology and delays. Under mild assumptions on the topology of the graph, our algorithm takes a time $O((\tau_{\max} + \Delta_{\max})\sqrt{\kappa/\gamma}\ln(\epsilon^{-1}))$ to reach a precision ϵ where γ is the spectral gap of the graph, $\tau_{\max}$ the maximum communication delay and $\Delta_{\max}$ the maximum computation time. Therefore, it matches the rate of SSDA, which is optimal when $\tau_{\max} = \Omega(\Delta_{\max})$. Applying our algorithm to quadratic local functions leads to an accelerated randomized gossip algorithm of rate $O(\sqrt{\theta_{\text{gossip}}/n})$ where θ_{gossip} is the rate of the standard randomized gossip. To the best of our knowledge, it is the first asynchronous gossip algorithm with a provably improved rate of convergence of the second moment of the error. We illustrate these results with experiments in idealized settings.

TAU Team

7. New Results

7.1. Toward Good AI

7.1.1. Causal Modeling

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag;
Post-docs and PhDs: Olivier Goudet, Diviyan Kalainathan
Collaboration: David Lopez-Paz (Facebook).

The search for **causal models** relies on quite a few hardly testable assumptions, e.g. causal sufficiency [152]; it is a data hungry task as it has the identification of independent and conditionally independent pairs of variables at its core. A new approach investigated through the Cause-Effects Pairs (CEP) Challenge [107] formulates causality search as a supervised learning problem, considering the joint distributions of pairs of variables (e.g. (Age, Salary)) labelled with the proper causation relationship between both variables (e.g. Age "causes" Salary) and learning algorithms apt to learn from distributions have been proposed [109]. An edited book is in preparation [64].

In D. Kalainathan's PhD and O. Goudet's postdoc, the search for causal models has been tackled in the framework of generative networks [44], trained to minimize the Maximum Mean Discrepancy loss; the resulting Causal Generative Neural Network improves on the state of the art on the CEP Challenge. However, due to the shortage of real-world variable pairs for which the causation type is known, the CEP challenge has been enriched using artificial pairs (e.g. considering variations on pairs of entities involved in biological regulatory networks), biasing the causation training process. On-going studies investigate how the use of such artificial pairs (the so-called Mother Distribution) to train a causation model aimed at real pairs can be cast as a domain adaptation problem [97], [78].

An attempt to circumvent the need for a large dataset of variable pairs, sampled for the Mother Distribution, we proposed the Structural Agnostic Model approach [57]. Working directly on the observational data, this global approach implements a variant of the popular adversarial game [97] between a discriminator, attempting to distinguish actual samples from fake ones, obtained by generating each variable, given real values from all others. A sparsity L_1 penalty forces all generators to consider only a small subset of their inpu variables, yielding a sparse causal graph. SAM obtains state-of-the-art performances on synthetic data.

An innovative usage of causal models is for educational training in sensitive domains, such as medicine, along the following line. Given a causal generative model, artificial data can be generated using a marginal distribution of causes; such data will enable students to test their diagnosis inference (with no misleading spurious correlations in principle), while forbidding to reverse-engineer the artificial data and guess the original data. Some motivating applications for causal modeling are described in section 4.1 .

7.1.2. Explainability

Participants: Isabelle Guyon, François Landes, Marc Schoenauer, Michèle Sebag.

Causal modeling is one particular method to tackle explainability, and TAU has been involved in other initiatives toward explainable AI systems. Following the LAP (Looking At People) challenges, Isabelle Guyon and co-organizers have edited a book [29] that presents a snapshot of explainable and interpretable models in the context of computer vision and machine learning. Along the same line, they propose an introduction and a complete survey of the state-of-the-art of the explainability and interpretability mechanisms in the context first impressions analysis [56].

The team is also involved in the proposal for the IPL HyAIAI (Hybrid Approaches for Interpretable AI), coordinated by the LACODAM team (Rennes) dedicated to the design of hybrid approaches that combine state of the art numeric models (e.g., deep neural networks) with explainable symbolic models, in order to be able to integrate high level (domain) constraints in ML models, to give model designers information on ill-performing parts of the model, and to provide understandable explanations on its results.

Finally, a completely original approach to DNN explainability might arise from the study of structural glasses (7.2.3), with a parallel to CNNs with rotational invariances, that could become an excellent non-trivial example for developing explainability protocols.

7.1.3. Experimental Validation of the Autonomous Vehicle

Participants: Guillaume Charpiat, Marc Schoenauer; **PhD and Engineers**: Marc Nabhan, Nizham Makhoud, Raphaël Jaiswal
Collaboration: Hiba Hage, Philippe Reynaud, and Yves Tourbier (Renault)

As said (Section 3.1.2 , TAU is considering two directions of research related to the certification of MLs. The first direction, toward experimental validation, focuses on the coverage of the datasets (more particularly here, used to train an autonomous vehicle controller), and is the subject of this section, while the second one, related to formal approaches, has just started with the beginning of Julien Girard's PhD and has not yet lead to results.

Statistical guarantees (e.g., less than 10^{-8} failure per hour of operation) are obtained by empirical tests, involving millions of kilometers of driving in all possible road, weather and traffic conditions as well as intensive simulations, the only way to full control of the driving conditions. The validation process thus involves 3 steps: i) making sure that all parts of the space of possible scenarios are covered by experiments/tests with sufficiently fine grain; ii) identify failures zones in the space of scenarios; iii) fix the controller flaws that resulted in these failures.

TAU is collaborating with Renault on steps i) (topic of a one-year POC) and ii) (Marc Nabhan's CIFRE PhD). In both cases, the current target scenario is the insertion of a car on a motorway, the "drosophila" of autonomous car scenarios.

Note that another approach toward experimental robustness is investigated in Nizam Makdoud's PhD (CIFRE Thalès), started in March 2018, where Reinforcement Learning is used to find ways to fool some security system.

Clustering of scenarios A first one-year Proof of Concept (ending Oct. 2018) has demonstrated the feasibility and the usefulness of scenario clustering, assuming the availability of data describing the scenarios, i.e., the trajectories of all vehicles involved. Publicly available datasets (e.g., NGSIM were used in a first step. The difficulties met are the following. Firstly, trajectories are varying-length time series, requiring the use of recurrent NNs or LSTMs. Secondly, a scenario is invariant under permutations of the different vehicles involved; neural architectures are taking inspiration from *social LSTMs* [67]. Lastly, most recorded real-world scenarios are uninteresting (all vehicles drive on in their lanes).

The results of this POC have been duly delivered to Renault, but will remain internal at this point. The follow-up collaboration will explore metrics (in the latent space, or learned via Siamese networks), to complete the clustering in a semi-supervised setting (exploiting human feedback to select "typical" scenarios).

Detection of controller flaws Marc Nabhan's PhD (CIFRE Renault) is concerned with the identification of the conditions of failures of the autonomous car controller. Only simulations are considered here, with one scenario being defined as a parameter setting of the in-house simulator SCANeR. The goal is the detection of as many failures as possible, running as few simulations as possible.

A key difficulty, beside that of getting actual data, is the very low probability of failure.On-going work builds upon TAU expertise in active learning using Monte-Carlo Tree Search [140] and evolutionary optimization, in particular taking inspiration from Novelty Search [121] to focus the exploration on unexplored regions of the scenario space, as well as portfolio optimization and instance-based algorithm selection (see Section 3.3.1).

7.2. Learning to Learn

*7.2.1. Auto-**

Participants: Guillaume Charpiat, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, François Gonard, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun, Pierre Wolinski
Collaboration: Vincent Renault (SME Artelys); Olivier Bousquet (Google Zurich), Yann Ollivier (Facebook)

TAU is an active player in the Auto-☆ field, having organized the sixth COSEAL workshop in Paris in September 2018. Furthermore, Auto-☆ studies at TAU investigate several directions.

As discussed in Section 3.3 , the most widely used approach is based on meta-features describing datasets, and builds upon past work in the team, such as Nacim Belkhir's PhD defended in 2017 [71], who won a GECCO competition in 2018 (Section 5.1.1), and François Gonard's PhD [11], defended in May 2018: an empirical performance model is built from the meta-features, and used to choose the best algorithm and its parameter configuration for unknown datasets. One key difficulty is to design useful meta-features: taking inspiration from equivariant learning [136] and learning from distributions [124], on-going work aims to learn such meta-features, based on the OpenML archive [153]. This extensive archive reports on the test predictive accuracy obtained by a few hundred algorithm configurations over a few thousand datasets.

Also mentioned in Section 3.3 , another popular approach for algorithm selection is collaborative filtering. Active learning was used on top of the CofiRank algorithm for matrix factorization [156], improving the results and the time to solution of the recommendation algorithm [62].

An original approach to Auto-☆, explored in Herilalaina Rakotoarison's PhD, extends and adapts Monte-Carlo Tree Search to explore the structured space of pre-processing + learning algorithm configurations, and gradually determine the best pipeline [40]; the resulting algorithm yields promising results comparatively to AutoSklearn. A difficulty consists in managing the exploration together with the resource allocation (considering subsampled datasets and/or limited computational resources in the early MCTS stages, akin [91]).

Most real-world domains evolve with time, and an important issue in real-world applications is that of life-long learning, as static models can rapidly become obsolete. An extension of AutoSklearn was proposed, part of Lisheng Sun's PhD, that detects concept drifts and corrects the current model accordingly [38].

Two on-going works focus on the specific adjustment of hyper-parameters for neural nets, deriving rules for the network architecture (Pierre Wolinski's PhD), or (Leonard Blier's PhD) attaching fixed learning rates to each neuron and calibrating the learning rate distribution in such a way that neurons are sequentially active, learning in an optimally agile manner during a given learning phase, and being stable in later phases.

A last direction of investigation concerns the design of challenges, that contribute to the collective advance of research in the Auto-☆ direction. The team has been very active in the series of AutoML challenges [42], and continuously contributes to the organization of new challenges (Section 7.6).

7.2.2. Deep Learning: Practical Theoretical Insights

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, Corentin Tallec
Collaboration: Yann Ollivier (Facebook AI Research, Paris), the Altschuler and Wu lab. (UCSF, USA)

Even though a full mathematical understanding of deep learning is not available today, theoretical insights from information theory or from dynamical systems can bring significant improvements to practical deep learning algorithms or offer strong explanations for the success of some architectures compared to others.

In [32] we fully derive the LSTM structure from first axiomatic principles, using an axiom of *robustness to temporal deformation (warpings) in the data*. The LSTM architecture, introduced in the 90's, has become the currently dominant architecture for modeling temporal sequences (such as text) in deep learning. But the LSTM architecture itself is quite complex and appears very much ad hoc at first sight. We prove that LSTMs necessarily arise if one wants the model to be able to handle time warpings in the data (such as arbitrary accelerations or decelerations in the signal). In fact, LSTM-like structures are the only way to provide robustness to such deformations: their complex equations can be derived axiomatically.

In [28] (long oral presentation at ICML) we tackle the problem of mode loss in generative models via information theory. The problem is to find generative models to produce more samples similar to samples in a dataset (eg, realistic images). The standard GAN approach is to couple a generative network and an adversary network whose job is to tell the differences between generated and genuine images. This suffers from mode loss: the generator focuses on doing some images well, rather than covering a full variety of images. Instead we propose to have the discriminator predict the proportion of true and fake images in a set of images, via an information theory criterion. This makes the discriminator work at the level of the *overall distribution* of images from the generator rather than individual images. By working on sets of images, the discriminator can detect statistical imbalances between different types of images created by the generator, thus reducing mode loss. An adapted architecture is derived for this, provably able to detect (in principle) all permutation-invariant statistics in a set of images.

In [43] we tackle the problem of recurrent network training via the theory of dynamical systems. Recurrent networks deal with temporal data sequences exhibiting temporal dependencies. Then backpropagation becomes backpropagation through time: for every new data point, training must rewind the network's computations backward in time on all past data to update the model parameters. This is unrealistic in any real-time application where the data arrive online. Two years ago we presented a fully online solution avoiding this "time rewind" step, based on real-time, noisy but unbiased approximations of model gradients. Our previous solution was mathematically well motivated but extremely complex to implement for standard models such as LSTMs. We now have a simpler variant which can be implemented easily in a black-box fashion on top of any recurrent model, and which is just as well-justified mathematically. The price to pay is more variance. In the long run, this could quite extend the applicability range of recurrent model to real-time situations.

In [31][0], we introduce a multi-domain adversarial learning algorithm in the semi-supervised setting. We extend the single source H-divergence theory for domain adaptation to the case of multiple domains, and obtain bounds on the average- and worst-domain risk in multi-domain learning. This leads to a new loss to accommodate semi-supervised multi-domain learning and domain adaptation. We obtain state-of-the-art results on two standard image benchmarks, and propose as a new benchmark a novel bioimage dataset, CELL, in the domain of automated microscopy data, where cultured cells are imaged after being exposed to known and unknown chemical perturbations, and in which each dataset displays significant experimental bias.

7.2.3. Analyzing and Learning Complex Systems

Participants: Cyril Furtlehner, Aurélien Decelle, François Landes
PhDs: Giancarlo Fissore
Collaboration: Jacopo Rocchi (LPTMS Paris Sud), the Simons team: Rahul Chako (post-doc), Andrea Liu (UPenn), David Reichman (Columbia), Giulio Biroli (ENS), Olivier Dauchot (ESPCI).
The information content of a trained restricted Boltzmann machine (RBM) for instance can be analyzed by comparing the singular values/vectors of its weight matrix, referred to as data modes, to that of a random RBM (typically following a Marchenko-Pastur distribution) [83]. The general strategy here is to replace the analysis of the learning process of a single instance by that of a well chosen statistical ensemble of models. In G. Fissore's PhD, the learning trajectory of an RBM is shown to start with a linear phase recovering the dominant modes of the data, followed by a non-linear regime where the interaction among the modes is characterized [15]. While the mean-field analysis conducted in closed form requires simplifying assumptions, it suggests some simple heuristics to speed up the convergence and to simplify the models. Ongoing works

[0] to be presented at ICLR 2019

concern extensions of these considerations to settings with missing input on the practical side and to the analysis of exactly solvable RBM - i.e. non-linear RBM for which the contrastive divergence can be computed in closed forms - on the theoretical side. Additionnally, we are collaborating with J. Rocchi, working at the LPTMS (Univ. Paris Sud), to investigate the landscape of RBMs learned from different initial conditions and to characterized it as a function of the number of parameters (hidden nodes) of the system.

A long standing application of our aforementioned mean-field inference methods based on probabilistic modelling concerns road traffic forecasting. In [49] we wrap up some of the techniques developed in these past works and perform, thanks to PTV-SISTeMA comprehensive experimental tests on various real world Urban traffic dataset in order to illustrate in various conditions the effectiveness of our method. As a by-product we show to some extent how to disentangle the model bias from errors caused by corrupted data and shed some light on the nature of the data themselves.

An emerging research topic, that we started to investigate thanks to exchanges with Lenka Zdeborova's group [96], is to revisit the Information Bottleneck framework [151] and analyze on non-toy NNs the gradual distillation of the mutual information (MI) along the NN layers, minimizing the MI with the input while preserving the MI with the sought output (the labels). More generally, information theory concepts could also be used to analyze the behavior of the network, for instance to detect adversarial attacks through unusual neural activity mapping.

As mentioned earlier, the use of ML to address fundamental physics problems is quickly growing. One example is the domain of glasses (how the structure of glasses is related to their dynamics), which is one of the major problems in modern theoretical physics. The idea is to let ML models automatically find the hidden structures (features) that control the flowing or non-flowing state of matter, discriminating liquid from solid states. These models could then help identifying "computational order parameters", that would advance the understanding of physical phenomena, on the one hand, and support the development of more complex models, on the other hand. Furthermore, this problem is new to the ML community and could provide an original non-trivial example for engineering, testing and benchmarking explainability protocols.

7.3. Computational Social Sciences

Computational Social Sciences (CSS) is making significant progress in the study of social and economic phenomena thank to the combination of social science theories and new insight from data science. But while the simultaneous advent of massive data and massive computational power has opened exciting new avenues, it has also raised new questions and challenges.

Almost ten years after the first enthusiasms for "big data" in social science, P. Tubaro has undertaken a reflective effort to look back at progress made so far and at directions for the near future. She edited a special issue of *Revue Française de Sociologie* on the effects of data both on society itself and on the scientific disciplines that engage with it [46], of which she co-authored the introduction [13].

Meanwhile, four data-based studies are being conducted in TAU, about labor (hiring, working on Internet, quality of life and economic performance), about nutrition (health, food, and socio-demographic issues), around Cartolabe, a platform for scientific information system and visual querying and around GAMA, a multi-agent based simulation platform.

7.3.1. Labor Studies

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag, Paola Tubaro
Post-docs; PhDs: Olivier Goudet; François Gonard, Diviyan Kalainathan, Thomas Schmitt
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Antonio Casilli (Telecom); Thierry Weil (Mines); Jean-Luc Bazet (RITM)

A first area of activity of TAU in Computational Social Sciences is the study of labor, from the functioning of the job market, to the rise of new, atypical forms of work in the networked society of internet platforms, and the quality of life at work.

Job markets Our first study in the domain of job markets (Th. Schmitt's and F. Gonard's PhDs [12], [11]) tackled the matching of job ads and CVs. This study, funded by the Lidex *Institut de la Société Numérique* (ISN) at Univ. Paris-Saclay, was conducted in collaboration with EHESS, on data provided by the hiring Web agency Qapa (for blue-collars and temporary jobs) and by Association Bernard Gregory (for scientists in industry). Among other difficulties, this study revealed that for both qualified and unqualified job sectors, job seekers and recruiters do not speak the same language [143]. This first study will be continued and extended along two directions: counterfactual analysis (*What would be my options if I had this additional skill ?*DATAIA project Vadore, coll. ENSAE and Pôle Emploi), and the recommendation of vocational training (BPI-PIA contract JobAgile, coll. EHESS and Qapa). Both projects start end 2018.

The platform economy and digital labor Another topic concerns the digital economy and the transformations of labor that accompany the current developments of AI. P. Tubaro has researched the so-called "sharing economy" and ideals of social change associated to the economic model of the platform [33]. However, the platform economy is also disrupting traditional industries. CNRS's MITI office has funded a research on the effects of online services for the restaurant sector (such as La Fourchette, Trip Advisor, Yelp) on working conditions and quality of service. This project involves P. Tubaro, P. Caillou and partners at Telecom ParisTech and Paris Dauphine University.

Ongoing research is exploring online platform labor and its linkages to the development of AI. In collaboration with A.A. Casilli (Telecom ParisTech), P. Tubaro has received funding to conduct research on this topic from the Union Force Ouvrière (OPLa project), from France Stratégie (a Prime Minister's service), and from MSH Paris-Saclay (DiPLab project). A recent grant from DARES (French Ministry of Labor) will enable exploring labor changes in B2B platforms (with O. Chagny of IRES, a unions-funded think-tank).

Quality of life at work. A study, funded by ISN, examined the relationship between the quality of life at work (QLW), and the economic performance of companies [113]. The management and economics literature has already established a correlation between QLW and economic performance [76]. The question that we are currently addressing regards the direction of causality: do profitable companies pay more attention to the QLW ? Or do companies paying attention to QLW tend to be more profitable ? This project (coll. RITM Univ. Paris-Sud, SES Telecom ParisTech, Ecole des Mines, La Fabrique de l'Industrie) combines data at the individual level (DARES, Ministère du Travail) and at the company level (Secafi); cutting-edge causality algorithms are applied to address the question, and handle confounder variables such as the sector of activity.

7.3.2. Health, food, and socio-demographic issues

Participants: Philippe Caillou, Michèle Sebag, Paola Tubaro
Post-docs; PhDs: Nayat Sanchez-Pi
Collaboration: Louis-Georges Soler, Olivier Allais (INRA)

Another area of activity concerns the relationships between eating practices, socio-demographic features and health.

The Nutriperso project (IRS Univ. Paris-Saclay, coll. INRA, CEA, CNRS, INSERM, Telecom ParisTech and Univ. Paris-Sud) aims to: i) determine the impact of food items on health (e.g., related to T2 diabetes); ii) identify alternative food items, admissible in terms of taste and budget, and better in terms of health; iii) emit personalized food recommendations (noting that general recommendations such as *Eat 5 fruit and vegetable per day* are hardly effective on the targeted populations. Based on the Kantar database, reporting the food habits of 20,000 households over 20 years, our challenge is to analyze the food purchases at an unprecedented fine-grained scale (at the barcode level), and to investigate the relationship between diets, socio-demographic features, and body mass index (BMI). The challenge also regards the direction of causality; while some diets are strongly correlated to high BMI, the question is to determine whether, e.g., sugar-free sodas are a cause, or a consequence of obesity, or both.

Previous research in this area included the study of eating disorders and their relationship to people's social network and usages of technology [18].

7.3.3. Scientific Information System and Visual Querying

Participants: Philippe Caillou, Michèle Sebag
Engineer: Anne-Catherine Letournel, Jonas Renault
Collaboration: Jean-Daniel Fekete (AVIZ, Inria Saclay)

A third area of activity concerns the 2D visualisation and querying of the scientific expertise in an institute/university, based on their scientific production, given as a set of articles (authors, title, abstract). The Cartolabe project started as an Inria ADT (coll. TAO and AVIZ, 2015-2017). It received a grant from CNRS (coll. TAU, AVIZ and HCC-LRI, 2018-2019). Further extension proposals, in collaboration with the department of bibliometry from Univ. Paris-Saclay, are under submission at the time of writing.

This project was initially devised as an open-source platform, aimed to answer burning questions, as the growth of academic organization prevents anyone from having a precise knowledge of who does what in the organization: Who is expert in a topic (described as a bag of words)? How are topics related? What are the rising topics? (see also Section 6.3)

Its development and the interaction with the beta-user scientists using it, increasingly raises new questions at the crossroad of human-centered computing, data visualization and machine learning: How to deal with poly-thematic researchers? How to take advantage of the fact that researchers have ideas about their relevant scientific neighborhood, and learn person-dependent metric?

7.3.4. Multi-Agent based simulation framework for social science

Participants: Philippe Caillou
Collaboration: Patrick Taillandier (INRA), Alexis Drogoul and Nicolas Marilleau (IRD), Arnaud Grignard (MediaLab, MIT), Benoit Gaudou (Université Toulouse 1)

Since 2008, P. Caillou contributes to the development of the GAMA platform, a multi-agent based simulation framework. Its evolution is driven by the research projects using it, which makes it very well suited for social sciences studies and simulations.

The 1.8 version of the platform[20] brings new capabilities required for social science research, such as High Performance Computing to explore the simulation, Co-Modeling to link projects, advanced agent architectures to model complex behaviors and advanced visualization to display nice 3D representations for exploration and presentations.

7.4. Energy Management

7.4.1. Power Grids Daily Management

Participants: Isabelle Guyon, Marc Schoenauer
PhDs: Benjamin Donnot, Balthazar Donon, Herilalaina Rakotoarison
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Olivier Teytaud (Facebook)

In the context of the Power Grid safety (Benjamin Donnot's CIFRE PhD with RTE, to be defended in February 2019), the goal is to assess in real time the so-called "(n-1)" safety (see Section 4.2) of possible recovery actions after some problem occurred somewhere on the grid. However, the simulator that allows to compute the power flows in the whole network is far too slow to simulate in real time all n-1 possible failures. A simplified simulator is also available, but its accuracy is too poor to give any good result. Deep surrogate models can be trained off-line, based on the results of the slow simulator, with high0enough accuracy, but training as many models as possible failures (i.e., n-1), obviously doesn't scale up: the topology of the grid must be an input of the learned model, allowing to instantly compute the power flows at least for grid configurations close to the usual running state of the grid. A standard approach is the one-hot encoding of the topology, where n additional boolean inputs are added to the neural network, encoding the presence or absence of each line. An original "guided dropout" approach was proposed [24], in which the topology directly acts on the connections of the deep network: a missing line suppresses some connections. However, whereas the standard dropout method disconnect random connections for every batch, in order to improve the generalization capacity of the

network, the "guided dropout" method removes some connections based on the actual topology of the network. THis approach is experimentaly validated against the above-mentionned approaches on small subsets of the French grid (up to 308 lines). Interestingly, and rather suprisingly, even though only examples with a single disconnected line are used in the training set, the learned model is able of some additive generalization, and predictions are also accurate enough in the case 2 lines are disconnected. The guided dropout approach was later robustified [23] by learning to rapidly rank higher order contingencies including all pairs of disconnected lines, in order to prioritize the cases where the slow simulator is run: Another neural network is trained to rank all (n-1) and (n-2) contingencies in decreasing order of presumed severity.

7.4.2. Local Grids Optimization, and the Modeling of Worst-case Scenarios

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Victor Berger, Herilalaina Rakotoarison; **Post-doc**: Berna Batu
Collaboration: Vincent Renaut (Artelys)

One of the goals of the ADEME Next project, in collaboration with SME Artelys (see also Section 4.2), is the sizing and capacity design of regional power grids. Though smaller than the national grid, regional and urban grids nevertheless raise scaling issues, in particular because many more fine-grained information must be taken into account for their design and predictive growth.

Provided accurate predictions of consumption (see below), off-the-shelf graph optimization algorithms can be used. Berna Batu is gathering different approaches, while Herilalaina Rakotoarison's PhD is concerned with the automatic tuning of their parameters (see Section 7.2.1 , and his original approach, at the moment applied to standard benchmarks [40], as well as to Artelys' home optimizer at large Knitro, and compared to the state-of-the-art in parameter tuning (confidential deliverable).

In order to get accurate consumption predictions, V. Berger's PhD tackles the identification of the peak of energy consumption, defined as the level of consumption that is reached during at least a given duration with a given probability, depending on consumers (profiles and contracts) and weather conditions. The peak identification problem is currently tackled using Monte-Carlo simulations based on consumer profile- and weather-dependent individual models, at a high computational cost. The challenge is to exploit individual models to train a generative model, aimed to sampling the collective consumption distribution in the quantiles with highest peak consumption.

7.5. Data-driven Numerical Modelling

7.5.1. High Energy Physics

Participants: Cécile Germain, Isabelle Guyon
PhD: Victor Estrade, Adrian Pol
Collaboration: D. Rousseau (LAL), M. Pierini (CERN)

The role and limits of simulation in discovery is the subject of V. Estrade's PhD, specifically uncertainty quantification and calibration, that is how to handle the systematic errors, arising from the differences ("known unknowns") between simulation and reality, coming from uncertainty in the so-called nuisance parameters. In the specific context of HEP analysis, where relatively numerous labelled data are available, the problem is at the crosspoint of domain adaptation and representation learning. We have investigated how to directly enforce the invariance w.r.t. the nuisance in the sought embedding through the learning criterion (tangent back-propagation) or an adversarial approach (pivotal representation). The results [25] contrast the superior performance of incorporating a priori knowledge on a well separated classes problem (MNIST data) with a real case setting in HEP, in relation with the Higgs Boson Machine Learning challenge [66]. More indirect approaches based on either incorporating variance reduction for the parameter of interest or constraining the representation in a variational auto-encoder farmework are currently considered.

Anomaly detection is the subject of A. Pol PhD. Reliable data quality monitoring is a key asset in delivering collision data suitable for physics analysis in any modern large-scale high energy physics experiment. [60] focuses on supervised and semi-supervised methods addressing the identification of anomalies in the data collected by the CMS muon detectors. The combination of DNN classifiers capable of detecting the known anomalous behaviors, and convolutional autoencoders addressing unforeseen failure modes has shown unprecedented efficiency, compared either to production solution or classical anomaly detection (one-class or I-Forest). The result has been included in the production suite of the CMS experiment at CERN.

The highly visible TrackML challenge is described in section 7.6 .

7.5.2. Remote Sensing Imagery

Participants: Guillaume Charpiat
Collaboration: Yuliya Tarabalka, Armand Zampieri, Nicolas Girard, Pierre Alliez (Titane team, Inria Sophia-Antipolis)

The analysis of satellite or aerial images has been a long-time ongoing topic of research, but the remote sensing community moved only very recently to a principled vision of the tasks in a machine learning perspective, with sufficiently large benchmarks for validation. The main topics are the segmentation of (possibly multispectral) remote sensing images into objects of interests, such as buildings, roads, forests, etc., and the detection of changes between two images of the same place taken at different moments. The main differences with classical computer vision is that images are large (covering whole countries, typically cut into 5000×5000 pixels tiles), containing many small, potentially similar objects (and not one big object per image), that every pixel needs to be annotated (w.r.t. assigning a single label to a full image), and that the ground truth is often not reliable (spatially mis-registered, missing new constructions).

This year, deep learning techniques took over classical approaches in most labs, adapting neural network architectures to the specifics of the tasks. This is due notably to the creation of several large scale benchmarks (including one by us [127] and, soon after, larger ones by GAFAM). A still ongoing issue is the ability to generalize across datasets (as urban and rural areas look different in different parts of the world, or even within the same country, e.g. roof types in France).

The task of segmenting satellite images comes together with the one of their registration with cadastral maps. Indeed, the ground truth in remote sensing benchmarks (cadastral maps) is often imperfect, due to spurious deformations. We tackle this issue by *learning* how to register images of different modalities (RGB pictures vs. binary cadastral maps). If one tries to predict, given an RGB photography and an associated cadastral map, the deformation that warps one onto the other, by outputting a 2D vector field indicating the predicted displacement of each pixel (which can be as large as ± 32 px), then the problem considered is too hard (32×32 possibilities for each pixel 2D displacement vector). Instead, we simplifly the problem by decomposing it in a cascade of increasing resolutions. The idea is that if one zooms out by a factor 32, while knowing that the maximum possible displacement is of magnitude 32 px, then at this low resolution one has to move pixels by at most 1 pixel. Learning the task at this low resolution is thus easy. When it is done, if we zoom in by a factor 2, thus reaching a resolution lower than the original one by a factor 16, then the maximum displacement is again of 1 pixel (since larger displacements have been dealt with at the previous scale). And so on. In the end, we train a multi-scale chain of neural networks (double U-nets) [34], and later combine it with a segmentation task [27] in order to benefit from multi-task training, known to improve results.

7.5.3. Space Weather Forecasting

Participants: Cyril Furtlehner, Michèle Sebag
PhD: Mandar Chandorkar
Collaboration: Enrico Camporeale (CWI)

Space Weather is broadly defined as the study of the relationships between the variable conditions on the Sun and the space environment surrounding Earth. Aside from its scientific interest from the point of view of fundamental space physics phenomena, Space Weather plays an increasingly important role on our technology-dependent society. In particular, it focuses on events that can affect the performance and reliability of space-borne and ground-based technological systems, such as satellite and electric networks that can be damaged by an enhanced flux of energetic particles interacting with electronic circuits.[0]

Since 2016, in the context of the Inria-CWI partnership, a collaboration between TAU and the Multiscale Dynamics Group of CWI aims to long-term Space Weather forecasting. The project is extremely timely, as the huge amount of (freely available) space missions data has not yet been systematically exploited in the current computational methods for space weather. Specifically, the goal is to take advantage of the data produced everyday by satellites surveying the sun and the magnetosphere, and more particularly to relate solar images and the quantities (e.g., electron flux, proton flux, solar wind speed) measured on the L1 libration point between the Earth and the Sun (about 1,500,000 km and 1 hour time forward of Earth). The project is very ambitious: the accurate prediction of e.g., geomagnetic storms, or solar wind speed from solar images, would represent a giant leap in the field. A challenge is to formulate such goals in terms of supervised learning problem, while the "labels" associated to solar images are recorded at L1 (thus with a varying and unknown time lag). In essence, while typical ML models aim to answer the question *What*, our goal here is to answer both questions *What* and *When*. Concerning the prediction of solar wind impacting earth magnetosphere from solar images, we encountered an interesting sub-problem related to the non deterministic travel time of a solar eruption to earth's magnetosphere. We have formalized it as the joint regression task of predicting the magnitude of signals as well as the time delay with respect to their driving phenomena and provided a solution tested on synthetic data.

7.5.4. Genomic Data and Population Genetics

Participants: Guillaume Charpiat, Flora Jay
PhD: Théophile Sanchez
Collaboration: TIMC-IMAG (Grenoble), Estonian Biocentre (Institute of Genomics, Tartu, Estonia)

Thanks to the constant improvement of DNA sequencing technology, large quantities of genetic data should greatly enhance our knowledge about evolution and in particular the past history of a population. This history can be reconstructed over the past thousands of years, by inference from present-day individuals: by comparing their DNA, identifying shared genetic mutations or motifs, their frequency, and their correlations at different genomic scales. Still, the best way to extract information from large genomic data remains an open problem; currently, it mostly relies on drastic dimensionality reduction, considering a few well-studied population genetics features.

On-going work at TAU, around Théophile Sanchez' PhD, co-supervised by G. Charpiat and Flora Jay, aims at extracting information from genomic data using deep neural networks; the key difficulty is to build flexible problem-dependent architectures, supporting transfer learning and in particular handling data with variable size. In collaboration with the Bioinfo group at LRI, we designed new generic architectures, that take into account DNA specificities for the joint analysis of a group of individuals, including its variable data size aspects [141]. In the short-term these architectures can be used for demographic inference; the longer-term goal is to integrate them in various systems handling genetic data (e.g., epidemiological statistics) or other biological sequence data. In collaboration with the Estonian Biocentre (Tartu, Estonia), applications will consider thousands of sequenced human genomes, and expand our knowledge of the past human history. To this aim Burak Yelmen (PhD student at the Estonian Biocentre) will visit the lab from February to April 2019. Indeed, TAU expertise regarding the methodologies of exploiting missing and noisy data, and the resulting modeling biases, can contribute to enhance these novel population genetics methods, particularly so for methods heavily relying on simulated data (thus potentially suffering from the *reality gap*).

[0] After a recent survey conducted by the insurance company Lloyd's, an extreme Space Weather event could produce up to $2.6 trillion in financial damage.

We also contributed to tess, a method for fast inference of population genetic structure, through a collaboration with TIMC-IMAG. This method analyses SNP data and estimates the admixture coefficients (that is, the probability that an individual belongs to different groups given the genetic data) via matrix factorization. The observed high dimensional genetic data are reduced automatically via the rank-k approximation of the matrix factorization and thereby highlight the latent structure of the data: the matrix factorization scores correspond to the admixture coefficients while the loadings give the genetic characteristics of each cluster. This method is faster than the hierarchical Bayesian models that we had previously developed and hence well suited for large NGS data. We participated in the tess3 R package, that implements this algorithm, facilitates the visualization of population genetic structure and the projection on maps [14]. We are currently adapting closely related algorithms to enable dimension reduction of temporal data with an application to paleogenomics.

7.5.5. Sampling molecular conformations

Participants: Guillaume Charpiat
PhD: Loris Felardos
Collaboration: Jérôme Hénin (IBPC), Bruno Raffin (InriAlpes)

Numerical simulations on massively parallel architectures, routinely used to study the dynamics of biomolecules at the atomic scale, produce large amounts of data representing the time trajectories of molecular configurations. The configuration space is high-dimensional (10,000+), hindering the use of standard data analytics approaches. The use of advanced data analytics to identify intrinsic configuration patterns could be transformative for the field.

The high-dimensional data produced by molecular simulations live on low-dimensional manifolds; the extraction of these manifolds will enable to drive detailed large-scale simulations further in the configuration space. Among the possible options are i) learning a parameterization of the local, low-dimensional manifold and performing a geometric extrapolation of the molecule trajectories; ii) learning a coarse description of the system and its dynamics, supporting a fast prediction of its evolution. In both cases, the states estimated from the time- or configuration-simplified models will be used for steering large scale simulations, thus accelerating the sampling of stable molecular conformations.

This task will be tackled by combining manifold learning (to find a relevant low-dimensional representation space) and reinforcement learning (for the efficient exploration of the space), taking inspiration from Graph Neural Networks [86]. On-going studies use Graph Auto-encoders to extract a meaningful representation of the conformation of molecules and to predict dynamics.

7.5.6. Storm trajectory prediction

Participants: Mo Yang, Guillaume Charpiat
Collaboration: Claire Monteleoni, Sophie Giffard-Roisin (LAL / Boulder University), Balazs Kegl (LAL)

Cyclones, hurricanes or typhoons all designate a rare and complex event characterized by strong winds surrounding a low pressure area. Their trajectory and intensity forecast, crucial for the protection of persons and goods, depends on many factors at different scales and altitudes. Additionally storms have been more numerous since the 1990s, leading to both more representative and more consistent error statistics.

Currently, track and intensity forecasts are provided by numerous guidance models. Dynamical models solve the physical equations governing motions in the atmosphere. While they can provide precise results, they are computationally demanding. Statistical models are based on historical relationships between storm behavior and other parameters [82]. Current national forecasts are typically driven by consensus methods able to combine different dynamical models.

Statistical models perform poorly compared to dynamical models, although they rely on steadily increasing data resources. ML methods have scarcely been considered, despite their successes in related forecasting problems [160]. A main difficulty is to exploit spatio-temporal patterns. Another difficulty is to select and merge data coming from heterogeneous sensors. For instance, temperature and pressure are real values on a 3D spatial grid, while sea surface temperature or land indication rely on a 2D grid, wind is a 2D vector field, while many indicators such as geographical location (ocean, hemisphere...) are just real values (not fields), and displacement history is a 1D vector (time). An underlying question regards the *innate* vs *acquired* issue, and how to best combine physical models with trained models. On-going studies, conducted in collaboration with S. Giffard-Roisin and C. Monteleoni (now Univ. Boulder), outperform the state-of-the-art in many cases [26], [36], [35].

7.5.7. Analyzing Brain Activity

Participants: Guillaume Charpiat
Collaboration: Hugo Richard, Bertrand Thirion (Parietal team, Inria Saclay / CEA)

With the goal of understanding brain functional architecture, the brain activity of ten subjects is recorded by an fMRI scanner, while they are watching movies (sequences of short pieces of real movies). The analysis of the ensuing complex stimulation streams proceeds by extracting relevant features from the stimuli and correlating the occurrence of these features with brain activity recorded simultaneously with the presentation of the stimuli. The analysis of video streams has been carried in [87] or [108] using a deep convolutional network trained for image classification. The question is then to build good descriptors of videos, possibly involving motion.

We consider a deep neural network trained for action recognition on the largest dataset available [115], and use its activations as descriptors of the input video. This provides deep representations of the watched movies, from an architecture that relies either on optical flow, or on image content, or both simultaneously. We then train a linear model to predict brain activity from these features. From the different layers of the deep neural networks, we build video representations that allow us to segregate (1) occipital and lateral areas of the visual cortex (reproducing the results of [108] and (2) foveal and peripheric areas of the visual cortex. We also introduce an effi- cient spatial compression scheme for deep video features that allows us to speed up the training of our predictive algorithm [41]. We show that our compression scheme outperforms PCA by a large margin.

7.6. Challenges

Participants: Cécile Germain, Isabelle Guyon, Michèle Sebag
PhD: Zhengying Liu, Lisheng Sun
Collaboration: D. Rousseau (LAL), Andre Elisseeff (Google Zurich), Jean-Roch Vilmant (CERN)

Following the highly successful ChaLearn **AutoML** Challenges (NIPS 2015 – ICML 2016 [106] – PKDD 2018 [45]), the **AutoDL** challenge [37], to be run in 2019, addresses the problem of tuning the hyperparameters of Deep Neural Networks, including the topology of the network itself. Co-sponsored by Google Zurich, it will require participants to upload their code on the Codalab platform.

In conjunction with AutoDL, we will organize a challenge in computer vision called **AutoCV**, to promote automatic machine learning for video processing, in collaboration with University of Barcelona. This will make use of the TAU GPU cluster.

Part of the HEP activities of the team, **TrackML** [30], [61] first phase was run and co-sponsored by Kaggle, until September 2018. The second phase is presently running on Codalab, and will end in March 2019. The challenge has been presented at WCCI [61] and NIPS [30]. I. Guyon and C. Germain are in the organizing committee, and M. Schoenauer is member of the Advisory Committee. The TAU team, in collaboration with CERN, has taken a leading role in stimulating both the ML and HEP communities to address the combinatorial complexity explosion created by the next generation of particle detectors.

Beyond the LAP (Looking At People) series of challenges (see details and references in Section 3.4), the domain of autonomous analysis of human behavior from multimodal information has recently gained momentum. We have been involved in two Special Issues dedicated to these topics, *The Computational Face*, in PAMI [17], and *Apparent Personality Analysis*, in IEEE Trans. on Affective Computing [16]. Two other challenges were organized at ICPR 2018, one about the information fusion task in the context of multi-modal image retrieval in social media, the other one regarding the inference of personality traits from written essays, including textual and handwritten information [29].

The **HADACA** project (EIT Health) aims to run a series of challenges to promote and encourage innovations in data analysis and personalized medicine. The data challenges will gather transdisciplinary instructors (researchers and professors), students, and health professionals (clinicians). The outcome of the data challenges should provide: i) analytical frameworks to bridge the gap between large dataset and personalized medicine in disease treatments and ii) innovative pedagogical methods to sensitize students to big data analysis in health. As a synergistic activity, TAU is also engaged in a collaboration with the Rensselaer Polytechnic Institute (RPI, New-York, USA) to use challenges in the classroom, as part of their health-informatics curriculum.

The **L2RPN** (Learning to Run a Power Network) project (coll. RTE) [39] addresses the difficult problem of using Reinforcement Learning to assist human operator in their daily tasks of maintaining the French Ultra-High Voltage grid safety while routing power without interruption. We are collaborating with O. Pietquin (Google Brain) to firm up the challenge protocol, largely inspired by AlphaGo and other RL challenges, like the NIPS 2017 “Learning to run” challenge.

It is important to introduce **challenges in ML teaching**. This has been done (and is on-going) in I. Guyon’s Licence and Master courses: some assignments to Master students are to design small challenges, which are then given to Licence students in labs, and both types of students seem to love it. Along similar line, F. Landes proposed a challenge in the context of S. Mallat’s course, at Collège de France.

CQFD Project-Team

6. New Results

6.1. 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 this paper, 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: Alexandre Genadot (Inria CQFD) and Romain Azaïs.

6.2. Estimation of the average number of continuous crossings for non-stationary non-diffusion processes

Assume that you observe trajectories of a non-diffusive non-stationary process and that you are interested in the average number of times where the process crosses some threshold (in dimension d = 1) or hypersurface (in dimension d $\geq$ 2). Of course, you can actually estimate this quantity by its empirical version counting the number of observed crossings. But is there a better way? In this paper, for a wide class of piecewise smooth processes, we propose estimators of the average number of continuous crossings of an hypersurface based on Kac-Rice formulae. We revisit these formulae in the uni-and multivariate framework in order to be able to handle non-stationary processes. Our statistical method is tested on both simulated and real data.

Authors: Alexandre Genadot (Inria CQFD) and Romain Azaïs.

6.3. ClustGeo: an R package for hierarchical clustering with spatial constraints

In this paper, 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 α 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-Simonet, Amaury Labenne and Jérôme Saracco (Inria CQFD).

6.4. Change-point detection for Piecewise Deterministic Markov Processes

We consider a change-point detection problem for a simple class of Piecewise Deterministic Markov Processes (PDMPs). A continuous-time PDMP is observed in discrete time and through noise, and the aim is to propose a numerical method to accurately detect both the date of the change of dynamics and the new regime after the change. To do so, we state the problem as an optimal stopping problem for a partially observed discrete-time Markov decision process taking values in a continuous state space and provide a discretization of the state space based on quantization to approximate the value function and build a tractable stopping policy. We provide error bounds for the approximation of the value function and numerical simulations to assess the performance of our candidate policy.

Authors: Alice Cleynen and Benoîte de Saporta (Inria CQFD).

6.5. A sharp first order analysis of Feynman–Kac particle models, Part I: Propagation of chaos

This article provides a new theory for the analysis of forward and backward particle approximations of Feynman–Kac models. Such formulae are found in a wide variety of applications and their numerical (particle) approximation is required due to their intractability. Under mild assumptions, we provide sharp and non-asymptotic first order expansions of these particle methods, potentially on path space and for possibly unbounded functions. These expansions allow one to consider upper and lower bound bias type estimates for a given time horizon n and particle number N; these non-asymptotic estimates are $O(n/N)$. Our approach is extended to tensor products of particle density profiles, leading to new sharp and non-asymptotic propagation of chaos estimates. The resulting upper and lower bound propagations of chaos estimates seem to be the first result of this kind for mean field particle models.

Authors: Pierre Del Moral (Inria CQFD) and Ajay Jasrab.

6.6. A sharp first order analysis of Feynman–Kac particle models, Part II: Particle Gibbs samplers

This article provides a new theory for the analysis of the particle Gibbs (PG) sampler (Andrieu et al., 2010). Following the work of Del Moral and Jasra (2017) we provide some analysis of the particle Gibbs sampler, giving first order expansions of the kernel and minorization estimates. In addition, first order propagation of chaos estimates are derived for empirical measures of the dual particle model with a frozen path, also known as the conditional sequential Monte Carlo (SMC) update of the PG sampler. Backward and forward PG samplers are discussed, including a first comparison of the contraction estimates obtained by first order estimates. We illustrate our results with an example of fixed parameter estimation arising in hidden Markov models.

Authors: Pierre Del Moral (Inria CQFD) and Ajay Jasrab.

6.7. Exponential mixing properties for time inhomogeneous diffusion processes with killing

We consider an elliptic and time-inhomogeneous diffusion process with time-periodic coefficients evolving in a bounded domain of RdRd with a smooth boundary. The process is killed when it hits the boundary of the domain (hard killing) or after an exponential time (soft killing) associated with some bounded rate function. The branching particle interpretation of the non absorbed diffusion again behaves as a set of interacting particles evolving in an absorbing medium. Between absorption times, the particles evolve independently one from each other according to the diffusion semigroup; when a particle is absorbed, another selected particle splits into two offsprings. This article is concerned with the stability properties of these non absorbed processes. Under some classical ellipticity properties on the diffusion process and some mild regularity properties of the hard obstacle boundaries, we prove an uniform exponential strong mixing property of the process conditioned to not be killed. We also provide uniform estimates w.r.t. the time horizon for the interacting particle interpretation of these non-absorbed processes, yielding what seems to be the first result of this type for this class of diffusion processes evolving in soft and hard obstacles, both in homogeneous and non-homogeneous time settings.

Authors: Pierre Del Moral (Inria CQFD) and Denis Villemonais.

6.8. Investigation of asymmetry in E. coli growth rate

The data we analyze derives from the observation of numerous cells of the bacterium Escherichia coli (E. coli) growing and dividing. Single cells grow and divide to give birth to two daughter cells, that in turn grow and divide. Thus, a colony of cells from a single ancestor is structured as a binary genealogical tree. At each node

the measured data is the growth rate of the bacterium. In this paper, we study two different data sets. One set corresponds to small complete trees, whereas the other one corresponds to long specific sub-trees. Our aim is to compare both sets. This paper is accessible to post graduate students and readers with advanced knowledge in statistics.

Authors: Bernard Delyon, Benoîte De Saporta (Inria CQFD), Nathalie Krell, Lydia Robert.

6.9. Design of estimators for restoration of images degraded by haze using genetic programming

Restoring hazy images is challenging since it must account for several physical factors that are related to the image formation process. Existing analytical methods can only provide partial solutions because they rely on assumptions that may not be valid in practice. This research presents an effective method for restoring hazy images based on genetic programming. Using basic mathematical operators several computer programs that estimate the medium transmission function of hazy scenes are automatically evolved. Afterwards, image restoration is performed using the estimated transmission function in a physics-based restoration model. The proposed estimators are optimized with respect to the mean-absolute-error. Thus, the effects of haze are effectively removed while minimizing overprocessing artifacts. The performance of the evolved GP estimators given in terms of objective metrics and a subjective visual criterion, is evaluated on synthetic and real-life hazy images. Comparisons are carried out with state-of-the-art methods, showing that the evolved estimators can outperform these methods without incurring a loss in efficiency, and in most scenarios achieving improved performance that is statistically significant.

Authors: Jose Enrique Hernandez-Beltran, Victor H.Diaz-Ramirez, Leonardo Trujillo and Pierrick Legrand (Inria CQFD).

6.10. Controlling IL-7 injections in HIV-infected patients

Immune interventions consisting in repeated injection are broadly used as they are thought to improve the quantity and the quality of the immune response. However, they also raised several questions that remains unanswered, in particular the number of injections to make or the delay to respect between different injections to acheive this goal. Practical and financial considerations add constraints to these questions, especially in the framework of human studies. We specifically focus here on the use of interleukine-7 (IL-7) injections in HIV-infected patients under antiretroviral treatment, but still unable to restore normal levels of CD4+ T lymphocytes. Clinical trials have already shown that repeated cycles of injections of IL-7 could help maintaining CD4+ T lymphocytes levels over the limit of 500 cells per microL, by affecting proliferation and survival of CD4+ T cells. We then aim at answering the question : how to maintain a patient's level of CD4+ T lymphocytes by using a minimum number of injections (ie optimizing the strategy of injections) ? Based on mechanistic models that were previously developed for the dynamics of CD4+ T lymphocytes in this context, we model the process by a piecewise deterministic Markov model. We then address the question by using some recently established theory on impulse control problem in order to develop a numerical tool determining the optimal strategy. Results are obtained on a reduced model, as a proof of concept : the method allows to defined an optimal strategy for a given patient. This method could applied to optimize injections schedules in clinical trials.

Authors: Chloé Pasin, François Dufour (Inria CQFD), Laura Villain, Huilong Zhang (Inria CQFD), Rodolphe Thiébaut.

6.11. Stochastic Control of Observer Trajectories in Passive Tracking with Acoustic Signal Propagation Optimization

The authors present in this study 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 minimise its own detection range perceived by the other targets. The signal

considered is acoustic propagation attenuation. This approach is based on dynamic programming of a finite horizon Markov decision process. A quantisation method is applied to fully discretise the problem and allows a numerically tractable solution. Different scenarios are considered. The authors suppose at first that the position and the velocity of the targets are known and in the second they suppose that they are unknown and estimated by a Kalman type filter in a context of passive tracking.

Authors: Huilong Zhang (Inria CQFD), Benoite de Saporta (Inria CQFD), Francois Dufour (Inria CQFD), Dann Laneuville and Adrien Nègre.

6.12. Computable approximations for average Markov decision processes in continuous time

In this paper we study the numerical approximation of the optimal long-run average cost of a continuous-time Markov decision process, with Borel state and action spaces, and with bounded transition and reward rates. Our approach uses a suitable discretization of the state and action spaces to approximate the original control model. The approximation error for the optimal average reward is then bounded by a linear combination of coefficients related to the discretization of the state and action spaces, namely, the Wasserstein distance between an underlying probability measure μ and a measure with finite support, and the Hausdorff distance between the original and the discretized actions sets. When approximating μ with its empirical probability measure we obtain convergence in probability at an exponential rate. An application to a queueing system is presented.

Authors: Jonatha Anselmi (Inria CQFD), François Dufour (Inria CQFD) and Tomás Prieto-Rumeau.

6.13. Zero-Sum Discounted Reward Criterion Games for Piecewise Deterministic Markov Processes

This papers deals with the zero-sum game 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 min?max 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: Oswaldo Costa and François Dufour (Inria CQFD) and Tomás Prieto-Rumeau.

6.14. Approximation of discounted minimax Markov control problems and zero-sum Markov games using Hausdorff and Wasserstein distances

This paper is concerned with a minimax control problem (also known as a robust Markov decision process (MDP) or a game against nature) with general state and action spaces under the discounted cost optimality criterion. We are interested in approximating numerically the value function and an optimal strategy of this general discounted minimax control problem. To this end, we derive structural Lipschitz continuity properties of the solution of this robust MDP by imposing suitable conditions on the model, including Lipschitz continuity of the elements of the model and absolute continuity of the Markov transition kernel with respect to some probability measure. Then, we are able to provide an approximating minimax control model with finite state and action spaces, and hence computationally tractable, by combining these structural properties with a suitable discretization procedure of the state space (related to a probabilistic criterion) and the action spaces (associated to a geometric criterion). Finally, it is shown that the corresponding approximation errors for the value function and the optimal strategy can be controlled in terms of the discretization parameters. These results are also extended to a two-player zero-sum Markov game.

Authors: François Dufour (Inria CQFD) and Tomás Prieto-Rumeau.

6.15. On the expected total cost with unbounded returns for Markov decision processes

We consider a discrete-time Markov decision process with Borel state and action spaces. The performance criterion is to maximize a total expected utility determined by unbounded return function. It is shown the existence of optimal strategies under general conditions allowing the reward function to be unbounded both from above and below and the action sets available at each step to the decision maker to be not necessarily compact. To deal with unbounded reward functions, a new characterization for the weak convergence of probability measures is derived. Our results are illustrated by examples.

Authors: François Dufour (Inria CQFD) and Alexandre Genadot (Inria CQFD).

6.16. Applying Genetic Improvement to a Genetic Programming library in C++

A young subfield of Evolutionary Computing that has gained the attention of many researchers in recent years is Genetic Improvement. It uses an automated search method that directly modifies the source code or binaries of a software system tofind improved versions based on some given criteria. Genetic Improvement has achieved notable results and the acceptance of several research communities, namely software engineering and evolutionary computation. Over the past 10 years there has been core publications on the subject, however, we have identified, to the best of our knowledge, that there is no work on applying Genetic Improvement to a meta-heuristic system. In this work we apply the GI framework called GISMO to the Beagle Puppy library version 0.1 in C++, a Genetic Programming system configured to perform symbolic regression on several benchmark and real-world problems. The objective is to improve the processing time while maintaining a similar or better test-fitness of the best individual produced by the unmodified Genetic Programming search. Results show that GISMO can generate individuals that present an improvement on those two key aspects over some problems, while also reducing the effects of bloat, one of the main issues in Genetic Programming.

Authors: Victor R. López-López, Leonardo Trujillo, Pierrick Legrand (Inria CQFD).

MATHRISK Project-Team

7. New Results

7.1. Risk management in finance and insurance

7.1.1. Control of systemic risk in a dynamic framework

Interconnected systems are subject to contagion in time of distress. Recent effort has been dedicated to understanding the relation between network topology and the scope of distress propagation. It is critical to recognize that connectivity is a result of an optimization problem of agents, who derive benefits from connections and view the associated contagion risk as a cost. In our previous works on the control of contagion in financial systems (see e.g. [80], [41], [5]), a central party, for example a regulator or government, seeks to minimize contagion. In [54], in contrast, the financial institutions themselves are the decision makers, and their decision is made before the shock, with a rational expectation on the way the cascade will evolve following the shock. We are extending these studies in a *dynamic* framework by allowing a recovery feature in the financial system during the cascade process, captured by introducing certain extent of growth of the banks' assets between each round of contagion.

7.1.2. Option pricing in financial markets with imperfections and default

A. Sulem, M.C. Quenez and R. Dumitrescu have studied robust pricing in an imperfect financial market with default. In this setting, the pricing system is expressed as a nonlinear g-expectation $\mathcal{E}^g$ induced by a nonlinear BSDE with nonlinear driver g and default jump (see [24]). The case of American options in this market model is treated in [19]. The incomplete market case is under study.

7.1.3. American options

With Giulia Terenzi, D. Lamberton has been been working on American options in Heston's model. They have 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). Their paper "Variational formulation of American option prices in the Heston model" [32] is now in minor revision for *SIAM Journal on Financial Mathematics*.

They also have some results on monotonicity and regularity properties of the price function.

D. Lamberton has also a paper on the binomial approximation of the American put, in which a new bound for the rate of convergence of the binomial approximation of the Black-Scholes American put price is derived [32].

Optimal stopping problems involving the maximum of a diffusion is currently under investigation. Partial results obtained by D. Lamberton and M. Zervos) enable them to treat reward functions with little regularity.

7.1.4. Monte-Carlo methods for the computation of the Solvency Capital Requirement (SCR) in Insurance

A. Alfonsi has obtained a grant from AXA Foundation on a Joint Research Initiative with a team of AXA France working on the strategic asset allocation. This team has to make recommendations on the investment over some assets classes as, for example, equity, real estate or bonds. In order to do that, each side of the balance sheet (assets and liabilities) is modeled in order to take into account their own dynamics but also their interactions. Given that the insurance products are long time contracts, the projections of the company's margins have to be done considering long maturities. When doing simulations to assess investment policies, it is necessary to take into account the SCR which is the amount of cash that has to be settled to manage the portfolio. Typically, the computation of the future values of the SCR involve expectations under conditional laws, which is greedy in computation time. The goal of this project is to develop efficient Monte-Carlo methods to compute the SCR for long investment strategies. A. Cherchali has started his PhD thesis in September 2017 on this topic.

A. Alfonsi and A. Cherchali are developing a model of the ALM management of insurance companies that takes into account the regulatory constraints on life-insurance. We are testing this model. The purpose is then to use this model to develop Monte-Carlo methods to approximate the SCR (Solvency Capital Requirement).

7.2. Optimal transport and applications

7.2.1. Martingale Optimal Transport.

B. Jourdain and W. Margheriti exhibit a new family of martingale couplings between two one-dimensional probability measures μ and ν in the convex order. This family is parametrised by two dimensional probability measures on the unit square with respective marginal densities proportional to the positive and negative parts of the difference between the quantile functions of μ and ν. It contains the inverse transform martingale coupling which is explicit in terms of the cumulative distribution functions of these marginal densities. The integral of $|x-y|$ with respect to each of these couplings is smaller than twice the W^1 distance between μ and ν. When the comonotoneous coupling between μ and ν is given by a map T, the elements of the family minimize $\int_{\mathbf{R}} |y-T(x)|M(dx,dy)$ among all martingale couplings M between μ and ν. When μ and ν are in the decreasing (resp. increasing) convex order, the construction can be generalized to exhibit super (resp. sub) martingale couplings.

A. Alfonsi and B. Jourdain show that any optimal coupling for the quadratic Wasserstein distance $W_2^2(\mu,\nu)$ between two probability measures μ and ν with finite second order moments on $\mathbf{R}^d$ is the composition of a martingale coupling with an optimal transport map $\mathcal{T}$. They check the existence of optimal couplings in which this map gives the unique optimal coupling between μ and $\mathcal{T}\#\mu$. Next, they prove that $\sigma \mapsto W_2^2(\sigma,\nu)$ is differentiable at μ in both Lions and the geometric senses iff there is a unique optimal coupling between μ and ν and this coupling is given by a map.

7.2.2. Numerical methods for optimal transport.

Optimal transport problems have got a recent attention in many different fields including physics, quantum chemistry and finance, where Martingale Optimal Transport problems allow to quantify the model risk. In practice, few numerical methods exist to approximate the optimal coupling measure and/or the optimal transport. In particular, to deal with large dimensions or with the optimal transport problems with many marginal laws, a natural direction is to develop Monte-Carlo methods.

A. Alfonsi, V. Ehrlacher (CERMICS, Inria Project-team MATHERIALS), D. Lombardi (Inria Project-team Reo) and R. Coyaud (PhD student of A. Alfonsi) are working on numerical approximations of the optimal transport between two (or more) probability measures.

7.3. Optimal Control of Mean field (S)PDEs

With Rui Chen and R. Dumitrescu, A. Sulem has studied mean-field Backward SDEs driven by a Brownian motion and an independant Poisson random measure and its interpretation in terms of global risk measures. Dual representation has been provided in the convex case. Optimal stopping for these BSDEs and links with reflected mean-field BSDEs has also been investigated.

A. Sulem, R. Dumitrescu and B. Øksendal have studied optimal control for mean-field stochastic **partial** differential equations (stochastic evolution equations) driven by a Brownian motion and an independent Poisson random measure, in the case of *partial information* control [20]. One important novelty is the introduction of *general mean-field* operators, acting on both the controlled state process and the control process. A sufficient and a necessary maximum principle for this type of control is formulated. Existence and uniqueness of the solution of such general forward and backward mean-field stochastic partial differential equations are proved. These results have been applied to find the explicit optimal control for an optimal harvesting problem.

7.4. Analysis of probabilistic numerical methods

7.4.1. Particles approximation of mean-field SDEs

O. Bencheikh and Benjamin Jourdain have proved that the weak error between a stochastic differential equation with nonlinearity in the sense of McKean given by moments and its approximation by the Euler discretization with time-step h of a system of N interacting particles is $\mathcal{O}(N^{-1}+h)$. Numerical experiments confirm this behaviour and show that it extends to more general mean-field interaction.

7.4.2. Approximation of Markov processes

V. Bally worked on general approximation schemes in total variation distance for diffusion processes in collaboration with his former Phd student Clément Rey [52] This work includes high order schemes as Victoir-Ninomya for example. Further development in this direction is under study in collaboration with A. Alfonsi. Moreover, in collaboration with his former Phd student V. Rabiet and with D. Goreac (University Paris Est Marne la Vallée), V. Bally is studying approximations schemes for Piecewise Deterministic Markov Processes (see [17], [51]). In this framework the goal is to replace small jumps by a Brownien component - such a procedure is popular for "usual" jump equations, but the estimate of the error in the case of PDMP's is much more delicate. A significant example is the Bolzmann equation [28].

7.4.3. High order approximation for diffusion processes

A. Alfonsi and V. Bally are working on a generic method to achieve any weak order of convergence for approximating SDEs.

7.4.4. Adaptive MCMC methods

The Self-Healing Umbrella Sampling (SHUS) algorithm is an adaptive biasing algorithm which has been proposed in order to efficiently sample a multimodal probability measure.

In [21], G. Fort, B. Jourdain, T. Lelièvre and G. Stoltz extend previous works [68], [66], [67] and study a larger class of algorithms where the target distribution is biased using only a fraction of the free energy and which includes a discrete version of well-tempered metadynamics.

SIMSMART Team

6. New Results

6.1. Objective 1 – Rare events simulation

In [16], we present a short historical perpective of the importance splitting approach to simulate and estimate rare events, with a detailed description of several variants. We then give an account of recent theoretical results on these algorithms, including a central limit theorem for Adaptive Multilevel Splitting (AMS). Considering the asymptotic variance in the latter, the choice of the importance function, called the reaction coordinate in molecular dynamics, is also discussed. Finally, we briefly mention some worthwhile applications of AMS in various domains.

Adaptive Multilevel Splitting (AMS for short) is a generic Monte Carlo method for Markov processes that simulates rare events and estimates associated probabilities. Despite its practical efficiency, there are almost no theoretical results on the convergence of this algorithm. In [15], we prove both consistency and asymptotic normality results in a general setting. This is done by associating to the original Markov process a level-indexed process, also called a stochastic wave, and by showing that AMS can then be seen as a Fleming-Viot type particle system. This being done, we can finally apply general results on Fleming-Viot particle systems that we have recently obtained.

Probability measures supported on submanifolds can be sampled by adding an extra momentum variable to the state of the system, and discretizing the associated Hamiltonian dynamics with some stochastic perturbation in the extra variable. In order to avoid biases in the invariant probability measures sampled by discretizations of these stochastically perturbed Hamiltonian dynamics, a Metropolis rejection procedure can be considered. The so-obtained scheme belongs to the class of generalized Hybrid Monte Carlo (GHMC) algorithms. In [21], we show here how to generalize to GHMC a procedure suggested by Goodman, Holmes-Cerfon and Zappa for Metropolis random walks on submanifolds, where a reverse projection check is performed to enforce the reversibility of the algorithm for large timesteps and hence avoid biases in the invariant measure. We also provide a full mathematical analysis of such procedures, as well as numerical experiments demonstrating the importance of the reverse projection check on simple toy examples.

Feynman-Kac semigroups appear in various areas of mathematics: non-linear filtering, large deviations theory, spectral analysis of Schrodinger operators among others. Their long time behavior provides important information, for example in terms of ground state energy of Schrodinger operators, or scaled cumulant generating function in large deviations theory. In [17], we propose a simple and natural extension of the stability of Markov chains for these non-linear evolutions. As other classical ergodicity results, it relies on two assumptions: a Lyapunov condition that induces some compactness, and a minorization condition ensuring some mixing. We show that these conditions are satisfied in a variety of situations. We also show that our technique provides uniform in the time step convergence estimates for discretizations of stochastic differential equations.

6.2. Objective 2 – High dimensional and advanced particle filtering

Existing filtering based structural health monitoring (SHM) algorithms assume constant noise environment which does not always conform to the reality as noise is hardly stationary. Thus to ensure optimal solution even with non-stationary noise processes, the assumed statistical noise models have to be updated periodically. [8] incorporates a modification in the existing Interacting Particle-Kalman Filter (IPKF) to enhance its detection capability in presence of non-stationary noise processes. To achieve noise adaptability, the proposed algorithm recursively estimates and updates the current noise statistics using the post-IPKF residual uncertainty in prediction as a measurement which in turn enhances the optimality in the solution as well. Further, this algorithm also attempts to mitigate the ill effects of abrupt change in noise statistics which most often

deteriorates/ diverges the estimation. For this, the Kalman filters (KF) within the IPKF have been replaced with a maximum Correntropy criterion (MCC) based KF that, unlike regular KF, takes moments beyond second order into consideration. A Gaussian kernel for MCC criterion is employed to define a correntropy index that controls the update in state and noise estimates in each recursive steps. Numerical experiments on an eight degrees-of-freedom system establish the potential of this algorithm in real field applications.

Standard filtering techniques for structural parameter estimation assume that the input force is either known 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, force must therefore also be estimated. In [5], the input force is considered to be an additional state that is estimated in parallel to the structural parameters. Two concurrent filters are employed for parameters and force respectively. For the parameters, an interacting Particle-Kalman filter is used to target systems with correlated noise. Alongside this, a second filter is used to estimate the seismic force acting on the structure. In the proposed algorithm, the parameters and the inputs are estimated as being conditional on each other, thus ensuring stability in the estimation. The proposed algorithm is numerically validated on a sixteen degrees-of-freedom mass-spring-damper system and a five-story building structure. The stability of the proposed filter is also tested by subjecting it to a sufficiently long measurement time history. The estimation results confirm the applicability of the proposed algorithm.

6.3. Objective 3 – Non-parametric inference

The forecasting and reconstruction of ocean and atmosphere dynamics from satellite observation time series are key challenges. While model-driven representations remain the classic approaches, data-driven representations become more and more appealing to benefit from available large-scale observation and simulation datasets. In [12], [13] and [4], we investigate the relevance of recently introduced neural network representations for the forecasting and assimilation of geophysical fields from satellite-derived remote sensing data. As a case-study, we consider satellite-derived Sea Surface Temperature time series off South Africa, which involves intense and complex upper ocean dynamics. Our numerical experiments report significant improvements in terms of reconstruction performance compared with operational and state-of-the-art schemes.

Data assimilation methods aim at estimating the state of a system by combining observations with a physical model. When sequential data assimilation is considered, the joint distribution of the latent state and the observations is described mathematically using a state-space model, and filtering or smoothing algorithms are used to approximate the conditional distribution of the state given the observations. The most popular algorithms in the data assimilation community are based on the Ensemble Kalman Filter and Smoother (EnKF/EnKS) and its extensions. In [14], we investigate an alternative approach where a Conditional Particle Filter (CPF) is combined with Backward Simulation (BS). This allows to explore efficiently the latent space and simulate quickly relevant trajectories of the state conditionally to the observations. We also tackle the difficult problem of parameter estimation. Indeed, the models generally involve statistical parameters in the physical models and/or in the stochastic models for the errors. These parameters strongly impact the results of the data assimilation algorithm and there is a need for an efficient method to estimate them. Expectation-Maximization (EM) is the most classical algorithm in the statistical literature to estimate the parameters in models with latent variables. It consists in updating sequentially the parameters by maximizing a likelihood function where the state is approximated using a smoothing algorithm. In this paper, we propose an original Stochastic Expectation-Maximization (SEM) algorithm combined to the CPF-BS smoother to estimate the statistical parameters. We show on several toy models that this algorithm provides, with reasonable computational cost, accurate estimations of the statistical parameters and the state in highly nonlinear state-space models, where the application of EM algorithms using EnKS is limited. We also provide a Python source code of the algorithm.

6.4. Objective 4 – Model reduction

In [19], [7], we propose new methodologies to decrease the computational cost of safe screening tests for LASSO. We first introduce a new screening strategy, dubbed "joint screening test", which allows the rejection of a set of atoms by performing one single test. Our approach enables to find good compromises between complexity of implementation and effectiveness of screening. Second, we propose two new methods to decrease the computational cost inherent to the construction of the (so-called) "safe region". Our numerical experiments show that the proposed procedures lead to significant computational gains as compared to standard methodologies.

Model-order reduction methods tackle the following general approximation problem: find an "easily-computable" but accurate approximation of some target solution h. In order to achieve this goal, standard methodologies combine two main ingredients: i) a set of problem-specific constraints; ii) some "simple" prior model on the set of target solutions. The most common prior model encountered in the literature assume that the target solution h is "close" to some low-dimensional subspace. Recently, several contributions have shown that refined prior models (based on a set of embedded approximation subspaces) may lead to enhanced approximation performance. Unfortunately, to date, no theoretical results have been derived to support the good empirical performance observed in these contributions. The goal of [18] is to fill this gap. More specifically, we provide a mathematical characterization of the approximation performance achievable by some particular "multi-space" decoder and emphasize that, in some specific setups, this "multi-space" decoder has provably better recovery guarantees than its standard counterpart based on a single approximation subspace.

In [20], we deal with the estimation of rare event probabilities using importance sampling (IS), where an *optimal* proposal distribution is computed with the cross-entropy (CE) method. Although, IS optimized with the CE method leads to an efficient reduction of the estimator variance, this approach remains unaffordable for problems where the repeated evaluation of the score function represents a too intensive computational effort. This is often the case for score functions related to the solution of parametric partial differential equations (PPDE) with random inputs. This work proposes to alleviate computation by adapting a score function approximation along the CE optimization process. The score function approximation is obtained by selecting the surrogate of lowest dimensionality, whose accuracy guarantees to pass the current CE optimization stage. The adaptation of the surrogate relies on certified upper bounds on the error norm. An asymptotic analysis provides some theoretical guarantees on the efficiency and convergence of the proposed algorithm. Numerical results demonstrate the gain brought by the adaptive method in the context of pollution alerts and a system modelled by a PPDE.

In [2], we deal with model order reduction of PPDE. We consider the specific setup where the solutions of the PPDE are only observed through a partial observation operator and address the task of finding a good approximation subspace of the solution manifold. We provide and study several tools to tackle this problem. We first identify the best worst-case performance achievable in this setup and propose simple procedures to approximate this optimal solution. We then provide, in a simplified setup, a theoretical analysis relating the achievable reduction performance to the choice of the observation operator and the prior knowledge available on the solution manifold.

In [3], 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; *(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 e.g. Proper Orthogonal Decomposition or Dynamic Mode Decomposition, can be revisited and recast within the probabilistic framework considered in this paper. We illustrate the performance of the proposed approach by numerical results obtained for a standard geophysical model.

6.5. Miscellaneous

In [22], we devise methods of variance reduction for the Monte Carlo estimation of an expectation of the type $\mathbb{E}[\phi(X, Y)]$, when the distribution of X is exactly known. The key general idea is to give each individual of a sample a weight, so that the resulting weighted empirical distribution has a marginal with respect to the variable X as close as possible to its target. We prove several theoretical results on the method, identifying settings where the variance reduction is guaranteed. We perform numerical tests comparing the methods and demonstrating their efficiency.

TOSCA Project-Team

5. New Results

5.1. 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, Émilie Soret, Denis Talay, Etienne Tanré, Milica Tomasevic, Denis Villemonais.

5.1.1. Published works and preprints

- M. Bossy, J. Fontbona (Universidad de Chile, Chile) and H. Olivero-Quinteros (CIMFAV, Valparaíso, Chile) analysed mathematical model for the collective behavior of a fully connected network of finitely many neurons. They obtained that the whole system synchronize, up to some error controlled by the channels noise level. The associated nonlinear McKean-Vlasov equation concentrates, as time goes to infinity, around the dynamics of a single Hodgkin-Huxley neuron with a chemical neurotransmitter channel [42].
- M. Bossy, A. Dupré, P. Drobinski, L. Violeau and C. Briard (Zephyr ENR) obtained advances in stochastic Lagrangian approach for atmospheric boundary layer simulation, on the analysis of an optimal rate of convergence for the particle approximation method, and on validation case with the simulation of a Zephyr ENR wind farm site of six turbines [36].
- M. Di Iorio (Marine Energy Research and Innovation Center, Santiago, Chile), M. Bossy, C. Mokrani (Marine Energy Research and Innovation Center, Santiago, Chile), and A. Rousseau obtained advances in stochastic Lagrangian approaches for the simulation of hydrokinetic turbines immersed in complex topography [33], [50].
- Together with M. Andrade-Restrepo (Univ. Paris Diderot) and R. Ferrière (Univ. Arizona and École Normale Supérieure), N. Champagnat studied deterministic and stochastic spatial eco-evolutionary dynamics along environmental gradients. This work focuses on numerical and analytical analysis of the clustering phenomenon in the population, and on the patterns of invasion fronts [40].
- N. Champagnat and J. Claisse (Ecole Polytechnique) studied the ergodic and infinite horizon controls of discrete population dynamics with almost sure extinction in finite time. This can either correspond to control problems in favor of survival or of extinction, depending on the cost function. They have proved that these two problems are related to the quasi-stationary distribution of the processes controled by Markov controls [16].
- N. Champagnat and B. Henry (Univ. Lille 1) 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 [17].
- N. Champagnat and D. Villemonais solved a general conjecture on the Fleming-Viot particle systems approximating quasi-stationary distributions (QSD): in cases where several quasi-stationary distributions exist, it is expected that the stationary distribution of the Fleming-Viot processes approaches a particular QSD, called minimal QSD. They proved that this holds true for general absorbed Markov processes with soft obstacles [48].
- N. Champagnat, K. Coulibaly-Pasquier (Univ. Lorraine) and D. Villemonais obtained general criteria for existence, uniqueness and exponential convergence in total variation to QSD for multi-dimensional diffusions in a domain absorbed at its boundary [37]. These results improve and simplify the existing results and methods.

- N. Champagnat and D. Villemonais obtained contraction properties in total variation of general penalized processes, including time-inhomogeneous Markov processes with absorption and Markov processes in varying environments [20]. Their method allows to improve significantly the former results of [62], [63].
- N. Champagnat and D. Villemonais studied with R. Schott (Univ. Lorraine) models of deadlocks in distributed systems. They use the approach developped recently by the first two authors to study quasi-stationary distributions in order to characterize and compute numerically the asymptotic behaviour of the deadlock time and the behaviour of the system before deadlock, both for discrete and for diffusion models [47].
- A. Lejay and A. Brault have followed their work on rough flow, which provides an unified framework to deal with the theory of rough paths from the points of view of flows. In particular, they have shown existence of flows even when the associated rough differential equations have multiple solutions [44], [45].
- A. Lejay and P. Pigato have provided an estimator of the diffusion and drift coefficients when they are discontinuous at a threshold. These estimators have been applied to financial data and exhibit leverage as well as mean-reversion effects on S&P 500 stocks' prices [57], [30]
- A. Lejay, L. Lenôtre and G. Pichot have proposed a new Monte Carlo method based on random exponential time steps to deal with discontinuous diffusions coefficients and drift [35], [56]
- A. Lejay, S. Haraketi and E. Haoula have shown how to construct a diffusion on the Sierpinski gasket lifted to the Heisenberg group [53].
- J. Bion-Nadal (Ecole Polytechnique) and D. Talay have pursued their work on 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 and can be expressed in terms of the solution to a stochastic control problem, which allows one to deduce a priori estimates or to obtain numerical evaluations: cf. [41]. This solution is now shown to exist and be smooth even in cases where the infinitesimal generators of the considered diffusion processes are not strongly elliptic.

  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? The objective being to select a model minimizing the above distance to a target model, the construction and analysis of an efficient stochastic algorithm are being in progress.
- In [60] D. Talay and M. Tomasevic have developed and analysed a new type of stochastic interpretation of the one-dimensional parabolic-parabolic 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. In [12] M. Tomasevic has proven that the two-dimensional parabolic-parabolic Keller-Segel system in the whole Euclidean space and the corresponding McKean-Vlasov stochastic differential equation are well-posed under some explicit conditions on the parameters of the model.
- D. Talay and M. Tomasevic are studying the well-posedness and the propagation of chaos of the particle system related to the two-dimensional parabolic-parabolic Keller-Segel system. The singularity of the interaction kernel being more critical than in the one-dimensional case, the preceding analysis [26] cannot be extended and a fully new methodology needs to be developed.
- V. Martin Lac, D. Talay and M. Tomasevic have worked on theoretical and algorithmic questions related to the simulation of the Keller–Segel particle systems. A preliminary version of a library has been developed.
- H. Olivero (Inria, now University of Valparaiso, Chile) and D. Talay have constructed and analysed an hypothesis test which helps to detect when the probability distribution of complex stochastic

simulations has an heavy tail and thus possibly an infinite variance. This issue is notably important when simulating particle systems with complex and singular McKean-Vlasov interaction kernels whick make it extremely difficult to get a priori estimates on the probability laws of the mean-field limit, the related particle system, and their numerical approximations. In such situations the standard limit theorems do not lead to effective tests. In the simple case of independent and identically distributed sequences the procedure developed this year and its convergence analysis are based on deep tools coming from the statistics of semimartingales.

- V. Martin Lac, H. Olivero-Quinteros and D. Talay have worked on theoretical and algorithmic questions related to the simulation of large particle systems under singular interactions and to critical numerical issues related to the simulation of independent random variables with heavy tails. A preliminary version of a library has been developed.
- 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 have ended their work on a mean-field game and shown the convergence of the joint density function of the controlled particle system. The construction of the limit has required the construction of suitable Sobolev spaces on sets of probability measures on Polish spaces.
- E. Tanré and Pierre Guiraud (Univ. of Valparaíso) have worked on the synchronization in a model of network of noisy biological neurons. Using a large deviation principle, they prove the stability of the synchronized state under stochastic perturbations. They also give a lower bound on the probability of synchronization for networks which are not initially synchronized. This bound shows the robustness of the emergence of synchronization in presence of small stochastic perturbations [25].
- E. Tanré, P. Grazieschi (Univ. Warwick), M. Leocata (Univ. Pisa), C. Mascart (Univ. Côte d'Azur), J. Chevallier (Univ. of Grenoble) and F. Delarue (Univ. Côte d'Azur) have extended the previous work [9] to sparse networks of interacting neurons. They have obtained a precise description of the limit behavior of the mean field limit according to the probability of (random) interactions between two individual LIF neurons [52].
- E. Tanré has worked with Nicolas Fournier (Sorbonne Université) 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 membrane potential is set to a minimum value v_{min}, 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_n. Between jumps, the potentials of the neurons are assumed to drift in $[v_{min}, \infty)$, according to some well-posed ODE. They prove the existence and uniqueness of a heuristically derived mean-field limit of the system when $n \to \infty$ [51].
- 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 [31].
- Q. Cormier and E. Tanré studied with Romain Veltz (team MATHNEURO) the long time behavior of a McKean-Vlasov SDE modeling a large assembly of neurons. A convergence to the unique (in this case) invariant measure is obtained assuming that the interactions between the neurons are weak enough. The key quantity in this model is the "firing rate": it gives the average number of jumps per unit of times of the solution of the SDE. They derive a non-linear Voltera equation satisfied by this rate. They used methods from integral equation to control finely the long time behavior of this firing rate [49].

- D. Villemonais collaborates with the Gerontology Service of CHRU Nancy on statistics of time evolution of telomere lengths in human blood cells. This is a collaboration with Anne Gégout Petit (IECL, Inria BIGS), Simon Toupance (CHRU Nancy), Eliane Albuisson (CHRU Nancy), Athanasios Benetos (CHRU Nancy), Daphnée Germain (Ecole des Mines de Nancy). They proposed in [32] a telomeric signature for human beings, stable along age evolution. Lionel Lenôtre works as a post-doc on this topic within the project GEENAGE of LUE.
- D. Villemonais studied with C. Coron (Univ. Paris-Saclay) and S. Méléard (École Polytechnique) the extinction probability before fixation for multi-dimensional models of Wright-Fisher type with mutations [21].
- In collaboration with E. Horton and A. Kyprianou (University of Bath), D. Villemonais studied the large-time asymptotic behaviour of the neutron transport equation in a three-dimensional domain [55]. This work is motivated by the simulation of the flow of particles in a nuclear tank.
- D. Villemonais studied with C. Mailler (University of Bath) the asymptotic behaviour of generalized measure-valued Polya urn models taking values in non-compact sets, using techniques from the theory of stochastic algorithms [58].

5.1.2. Other works in progress

- N. Champagnat, C. Fritsch and S. Billiard (Univ. Lille) are working on food web modeling.
- N. Champagnat and D. Villemonais are working with M. Benaïm (Univ. Neuchatel) on the convergence of stochastic algorithms to the quasi-stationary distribution of diffusion processes absorbed at the boundary of a domain.
- N. Champagnat is working with S. Méléard (École Polytechnique) and C. Tran Viet (Univ. Lille 1) on evolutionary models of bacteria with horizontal transfer. They study a scaling of parameters taking into account the influence of negligible but non-extinct populations, allowing to study specific phenomena observed in these models (re-emergence of traits, cyclic evolutionary dynamics and evolutionary suicide).
- Q. Cormier is investigating new methods to explore the long time behavior of the McKean-Vlasov SDE of [49], to go beyond the weak interactions case. The long time behavior of such McKean-Vlasov equations can be intricate as there can be multiple invariant measures or stable oscillations of the law of the process. The objective of this work is to develop (numerical and theoretical) methods to check the local stability of a given invariant measure of this non-linear SDE.
- C. Fritsch is working with A. Gégout-Petit (Univ. Lorraine and EPI BIGS), B. Marçais (INRA, Nancy) and M. Grosdidier (INRA, Avignon) on a statistical analysis of a Chalara Fraxinea model [34].
- C. Fritsch is working with Marianne Clausel (Univ. Lorraine) and Julien Trombini (Two-I) on the modeling of emotions spreading in a crowd.
- A. Lejay and A. Brault (U. Paris Descartes) continue their work to extend the framework of rough flows.
- O. Faugeras (MATHNEURO Inria Research Team), É. Soret (joint postdoc with MATHNEURO Inria Research Team) and É. Tanré are working on Mean-Field description of thermodynamics limits of large population of neurons with random interactions. They study the asymptotic behaviour for an asymmetric neuronal dynamics in a network of linear Hopfield neurons. They obtain the convergence in law of each component to a Gaussian process. The limit object is not a Markov process.
- P. Helson, E. Tanré and R. Veltz (MATHNEURO Inria team), are working on a neural network model of memory. The aim is to propose a new retrieval criterion and its mathematical analysis.
- E. Tanré has worked 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 where 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.