RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

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Section New Results

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ACUMES Project-Team

6. New Results

6.1. Macroscopic traffic flow models on networks

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Bounded acceleration. In [50], we study a mathematical model accounting for the boundedness of traffic acceleration at a macroscopic scale that was introduced in [137]. 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 propose a Wave Front Tracking Algorithm to construct approximate solutions. We use this algorithm to prove the existence of solutions to the associated Cauchy Problem, and provide some numerical examples illustrating the solution behaviour.
This work was part of N. Laurent-Brouty's PhD thesis.

Moving bottlenecks on road networks. In [48], we generalize the Lighthill-Witham-Richards model for vehicular traffic coupled with moving bottlenecks introduced in [6] to the case of road networks. Such models can be applied to study the traffic evolution in the presence of a slow-moving vehicle, like a bus. At last, a numerical experiment is shown.
This work was part of N. Dymski's PhD thesis.

Traffic control by autonomous vehicles. Autonomous vehicles (AVs) allow new ways of regulating the traffic flow on road networks. Most of available results in this direction are based on microscopic approaches, where ODEs describe the evolution of regular cars and AVs. In [49], we propose a multiscale approach, based on recently developed models for moving bottlenecks. Our main result is the proof of existence of solutions for open-loop controls with bounded variation.

Vehicle platooning in highway traffic. In [52], we consider a model describing the presence of a platoon of vehicles moving in the traffic flow. The model consists of a coupled PDE-ODE system describing the interaction between the platoon and the surrounding traffic flow. The scalar conservation law takes into account the main traffic evolution, while the ODEs describe the trajectories of the initial and final points of the platoon, whose length can vary in time. The presence of the platoon acts as a road capacity reduction, resulting in a space-time discontinuous flux function. We describe the solutions of Riemann problems and design a finite volume numerical scheme sharply capturing non-classical discontinuities. Some numerical tests are presented to show the effectiveness of the method.
This work is part of G. Piacentini's PhD thesis.

Well-posedness of conservation laws on networks with finite buffers. In [51], we introduce a model dealing with conservation laws on networks and coupled boundary conditions at the junctions. In particular, we introduce buffers of fixed arbitrary size and time dependent split ratios at the junctions, which represent how traffic is routed through the network, while guaranteeing spill-back phenomena at nodes. Having defined the dynamics at the level of conservation laws, we lift it up to the Hamilton-Jacobi (H-J) formulation and write boundary datum of incoming and outgoing junctions as functions of the queue sizes and vice-versa. The Hamilton-Jacobi formulation provides the necessary regularity estimates to derive a fixed-point problem in a proper Banach space setting, which is used to prove well-posedness of the model. Finally, we detail how to apply our framework to a non-trivial road network, with several intersections and finite-length links.
This work was realized in the framework of the IIP ORESTE and was part of N. Laurent-Brouty's PhD thesis.

Traffic flow on multi-lane networks. In [28], we prove the well-posedness of a system of balance laws describing macroscopically the traffic flow on a multi-lane road network. Motivated by real applications, we allow for the the presence of space discontinuities both in the speed law and in the number of lanes. This allows to describe a number of realistic situations. Existence of solutions follows from compactness results on a sequence of Godunov's approximations, while L^1-stability is obtained by the doubling of variables technique. Some numerical simulations illustrate the behaviour of solutions in sample cases.

Minimum time boundary controls. The paper [35] is motivated by the practical problem of controlling traffic flow by imposing restrictive boundary conditions. For a one-dimensional congested road segment, we study the minimum time control problem of how to control the upstream vehicular flow appropriately to regulate the downstream traffic into a desired (constant) free flow state in minimum time. We consider the Initial-Boundary Value Problem (IBVP) for a scalar nonlinear conservation law, associated to the Lighthill-Whitham-Richards (LWR) Partial Differential Equation (PDE), where the left boundary condition, also treated as a valve for the traffic flow from the upstream, serves as a control. Besides, we set absorbing downstream boundary conditions. We prove first a comparison principle for the solutions of the considered IBVP, subject to comparable initial, left and right boundary data, which provides estimates on the minimal time required to control the system. Then we consider a (sub-) optimal control problem and we give numerical results based on Godunov scheme. The article serves as a starting point for studying time-optimal boundary control of the LWR model and for computing numerical results.
This work was realized in the framework of the IIP ORESTE.

Impact of on-line navigation devices in traffic flows. In [34], we consider a macroscopic multi-population traffic flow model on networks accounting for the presence of drivers (or autonomous vehicles) using navigation devices to minimize their instantaneous travel cost to destination. The strategic choices of each population differ in the degree of information about the system: while part of the agents knows only the structure of the network and minimizes the traveled distance, others are informed of the current traffic distribution, and can minimize their travel time avoiding the most congested areas. In particular, the different route choices are computed solving eikonal equations on the road network and they are implemented at road junctions. The impact on traffic flow efficiency is illustrated by numerical experiments. We show that, even if the use of routing devices contributes to alleviate congestion on the whole network, it also results in increased traffic on secondary roads. Moreover, the generalized use of real-time information can even deteriorate the efficiency of the network.

Uncertainty quantification in a macroscopic traffic flow model calibrated on GPS data. In [18], we analyze the inclusion of one or more random parameters into the deterministic Lighthill-Whitham-Richards traffic flow model and use a semi-intrusive approach to quantify uncertainty propagation. To verify the validity of the method, we test it against real data coming from vehicle embedded GPS systems, provided by AUTOROUTES TRAFIC.

6.2. Non-local conservation laws

Participants: Felisia Angela Chiarello, Paola Goatin, Elena Rossi, Jan Friedrich [U Mannheim, Germany], Simone Göttlich [U Mannheim, Germany], Jennifer Kotz [U Mannheim, Germany], Luis Miguel Villada [U Bìo-Bìo, Chile].

F.A. Chiarello's PhD thesis focused on non-local conservation laws. In [23], 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 [22], 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 has been published [24]. Besides, high-order numerical schemes for the same model were proposed in [78].
Finally, in [21], we present a model for a class of non-local conservation laws arising in traffic flow modeling at road junctions. Instead of a single velocity function for the whole road, we consider two different road segments, which may differ for their speed law and number of lanes (hence their maximal vehicle density). We use an upwind type numerical scheme to construct a sequence of approximate solutions and we provide uniform L^∞ and total variation estimates. In particular, the solutions of the proposed model stay positive and below the maximum density of each road segment. Using a Lax-Wendroff type argument and the doubling of variables technique, we prove the well-posedness of the proposed model. Finally, some numerical simulations are provided and compared with the corresponding (discontinuous) local model.

Besides, in [31], we focus on finite volume approximation schemes to solve a non-local material flow model in two space dimensions. Based on the numerical discretisation with dimensional splitting, we prove the convergence of the approximate solutions, where the main difficulty arises in the treatment of the discontinuity occurring in the flux function. In particular, we compare a Roe-type scheme to the well-established Lax-Friedrichs method and provide a numerical study highlighting the benefits of the Roe discretisation. We also prove the L^1-Lipschitz continuous dependence on the initial datum, ensuring the uniqueness of the solution.

6.3. Isogeometric Discontinuous Galerkin method for compressible flows

Participants: Régis Duvigneau, Stefano Pezzano, Maxime Stauffert.

The co-existence of different geometrical representations in the design loop (CAD-based and mesh-based) is a real bottleneck for the application of design optimization procedures in industry, yielding a major waste of human time to convert geometrical data. Isogeometric analysis methods, which consists in using CAD bases like NURBS in a Finite-Element framework, were proposed a decade ago to facilitate interactions between geometry and simulation domains.

We investigate the extension of such methods to Discontinuous Galerkin (DG) formulations, which are better suited to hyperbolic or convection-dominated problems. Specifically, we develop a DG method for compressible Euler and Navier-Stokes equations, based on rational parametric elements, that preserves exactly the geometry of boundaries defined by NURBS, while the same rational approximation space is adopted for the solution [37]. The following research axes are considered in this context:

- **Adaptive refinement**
  Properties of NURBS functions are used to define an adaptive refinement strategy, which refines locally the discretization according to an error indicator, while describing exactly CAD geometries whatever the refinement level. The resulting approach exhibits an optimal convergence rate and capture efficiently local flow features, like shocks or vortices, avoiding refinement due to geometry approximation [36], [47].
- **Arbitrary Eulerian-Lagrangian formulation**
  To enable the simulation of flows around moving bodies, an Arbitrary Eulerian-Lagrangian (ALE) formulation is proposed in the context of the isogeometric DG method. It relies on a NURBS-based boundary velocity, integrated along time over moving NURBS elements. The gain of using exact-geometry representations is clearly quantified [39].
- **Isogeometric shape optimization**
  On the basis of the isogeometric DG method, we develop a shape optimization procedure with sensitivity analysis, entirely based on NURBS representations [40]. The mesh, the shape parameters as well as the flow solutions are represented by NURBS, which avoids any geometrical conversion and allows to exploit NURBS properties, like regularity, hierarchy, etc.

6.4. Sensitivity analysis for unsteady flows

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

The adjoint equation method, classically employed in design optimization to compute functional gradients, is not well suited to complex unsteady problems, because of the necessity to solve it backward in time. Therefore, we investigate the use of the sensitivity equation method, which is integrated forward in time, in the context of compressible flows. More specifically, the following research axes are considered:

- **Sensitivity analysis in presence of shocks**
  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 1D compressible Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach. Applications to uncertainty quantification in presence of shocks are demonstrated and compared to the classical Monte-Carlo method [26]. This study is achieved in collaboration with C. Chalons and C. Fiorini from University of Versailles.
- **High-order derivatives**
  For problems with regular solution, we investigate the recursive use of the sensitivity equation method to estimate high-order derivatives of the solution with respect to parameters of interest. Such derivatives provide useful information for optimization or uncertainty quantification. More precisely, the third-order derivatives of flow solutions governed by 2D compressible Navier-Stokes equations are estimated with a satisfactory accuracy.
- **Shape sensitivity analysis**
  When shape parameters are considered, the evaluation of flow sensitivities is more difficult, because equations include an additional term, involving flow gradient, due to the fact that the parameter affects the boundary condition location. To overcome this difficulty, we propose to solve sensitivity equations using an isogeometric Discontinuous Galerkin (DG) method, which allows to estimate accurately flow gradients at boundary and consider boundary control points as shape parameters. First results obtained for 2D compressible Euler equations exhibit a sub-optimal convergence rate, as expected, but a better accuracy with respect to a classical DG method [40].

6.5. Optimization of nano-photonic devices

Participants: Mickaël Binois, Régis Duvigneau, Mahmoud Elsawy [NACHOS team], Alexis Gobé [NACHOS team], Stéphane Lanteri [NACHOS team].

In collaboration with NACHOS Project-Team, we consider the optimization of optical meta-surface devices, which are able to alter light properties by operating at nano-scale. In the contexte of Maxwell equations, modified to account for nano-scale phenomena, the geometrical properties of materials are optimized to achieve a desired electromagnetic wave response, such as change of polarization, intensity or direction. This task is especially challenging due to the computational cost related to the 3D time-accurate simulations and the difficulty to handle the different geometrical scales in optimization.

A first study, comparing an evolution strategy and a Bayesian optimization algorithm, demonstrates the potentiality of the proposed approach [25], [38].

6.6. Sequential learning of active subspace

Participants: Mickaël Binois, Nathan Wycoff [Virginia Tech], Stefan Wild [ANL].

Continuing a work started at Argonne National Laboratory, in [53] we consider the combination of Gaussian process regression modeling with the active subspace methods (ASMs), which have become a popular means of performing subspace sensitivity analysis on black-box functions. Naively applied, however, ASMs require gradient evaluations of the target function. In the event of noisy, expensive, or stochastic simulators, evaluating gradients via finite differencing may be infeasible. In such cases, often a surrogate model is employed, on which finite differencing is performed. When the surrogate model is a Gaussian process, we show that the ASM estimator is available in closed form, rendering the finite-difference approximation unnecessary. We use our closed-form solution to develop acquisition functions focused on sequential learning tailored to sensitivity analysis on top of ASMs. We also show that the traditional ASM estimator may be viewed as a method of moments estimator for a certain class of Gaussian processes. We demonstrate how uncertainty on Gaussian process hyperparameters may be propagated to uncertainty on the sensitivity analysis, allowing model-based confidence intervals on the active subspace. Our methodological developments are illustrated on several examples.

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

Participants: Mickaël Binois, Victor Picheny [Prowler.io], Abderrahmane Habbal.

Extending the short paper [67] on the use of the game-theoretic Kalai-Smorodinski solution in Bayesian optimization, we have refined the definition of solutions, discussed underlying assumptions, and shown empirically the improved performance of our proposed approach over naive heuristics. A realistic hyperparameter tuning problem with eight objectives as well as an expensive calibration problem with nine objectives have been considered as well.

In parallel, we have substantially improved the efficiency of the implementation, enabled specific treatment of calibration problems as well as handling noise in the `GPGame` package https://cran.r-project.org/web/packages/GPGame.

6.8. Heteroskedastic Gaussian process modeling and sequential design

Participants: Mickaël Binois, Robert Gramacy [Virginia Tech].

An increasing number of time-consuming simulators exhibit a complex noise structure that depends on the inputs. For conducting studies with limited budgets of evaluations, new surrogate methods are required in order to simultaneously model the mean and variance fields. To this end, in [43] we present the `hetGP` package https://cran.r-project.org/web/packages/hetGP, implementing many recent advances in Gaussian process modeling with input-dependent noise. First, we describe a simple, yet efficient, joint modeling framework that relies on replication for both speed and accuracy. Then we tackle the issue of data acquisition leveraging replication and exploration in a sequential manner for various goals, such as for obtaining a globally accurate model, for optimization, or for contour finding. Reproducible illustrations are provided throughout.

6.9. Direct and adaptive approaches to multi-objective optimization

Participants: Jean-Antoine Désidéri, Régis Duvigneau.

We formulate in a unified way the major theoretical results obtained by the authors in the domain of multi-objective differential optimization, discuss illustrative examples, and present a brief discussion of the related software developments made at Inria. The development is split in two connected parts. In Part A, the Multiple Gradient Descent Algorithm (MGDA), referred to as the direct approach, is a general construction of a descent method in the multi-objective optimization context. The algorithm provides a technique for determining Pareto optimal solutions in constrained problems as an extension of the classical steepest-descent method. In Part B, another problematics is posed, referred to as the adaptive approach. It is meant to be developed after a Pareto-optimal solution with respect to a set of primary cost functions subject to constraints has been elected in a first phase of optimization carried out by application of MGDA, or another effective multi-objective optimization technique, possibly an evolutionary strategy. This second phase of optimization permits to construct a continuum of neighboring solutions for which novel cost functions, designated as secondary cost functions, are reduced at the cost of a moderate degradation of the Pareto-stationarity condition of the primary cost functions. In this way, the entire optimization process demonstrates a form of adaptivity to the result of the first phase [42].

6.10. Platform for prioritized multi-objective optimization

Participant: Jean-Antoine Désidéri.

A multi-objective differentiable optimization algorithm had been proposed to solve problems presenting a hierarchy in the cost functions, $\{f_j(\mathbf{x})\}$ ($j = 1, \cdots, M \geq 2;\ \mathbf{x} \in \Omega_a \subseteq \mathsf{R}^n$). The first cost functions for which $j \in \{1, \cdots, m\}$ ($1 \leq m < M$) are considered to be of preponderant importance; they are referred to as the "primary cost functions" and are subject to a "prioritized" treatment, in contrast with the tail ones, for which $j \in \{m+1, \cdots, M\}$, referred to as the "secondary cost functions". The problem is subject to the nonlinear constraints, $c_k(\mathbf{x}) = 0$ ($k = 1, \cdots, K$). The cost functions $\{f_j(\mathbf{x})\}$ and the constraint functions $\{c_k(\mathbf{x})\}$ are all smooth, say $C^2(\Omega_a)$. The algorithm was first introduced in the case of two disciplines ($m = 1$, $M = 2$), and successfully applied to optimum shape design optimization in compressible aerodynamics concurrently with a secondary discipline [101] [105]. An initial admissible point $\mathbf{x}_A^{\star}$ that is Pareto-optimal with respect to the sole primary cost functions (subject to the constraints) is assumed to be known. Subsequently, a small parameter $\varepsilon \in [0, 1]$ is introduced, and it is established that a continuum of Nash equilibria $\{\overline{\mathbf{x}}_\varepsilon\}$ exists for all small enough ε. The continuum originates from $\mathbf{x}_A^{\star}$ ($\overline{\mathbf{x}}_0 = \mathbf{x}_A^{\star}$). Along the continuum: (*i*) the Pareto-stationarity condition exactly satisfied by the primary cost functions at $\mathbf{x}_A^{\star}$ is degraded by a term $O(\varepsilon^2)$ only, whereas (*ii*) the secondary cost functions initially decrease, at least linearly with ε with a negative derivative provided by the theory. Thus, the secondary cost functions are reduced while the primary cost functions are maintained to quasi Pareto-optimality. In this report, we firstly recall the definition of the different steps in the computational Nash-game algorithm assuming the functions all have known first and second derivatives (here without proofs). Then we show how, in the absence of explicitly known derivatives, the continuum of Nash equilibria can be calculated approximately via the construction of quadratic surrogate functions. Numerical examples are provided and commented [41].

6.11. Non-convex multiobjective optimization under uncertainty: a descent algorithm. Application to sandwich plate design and reliability

Participants: Quentin Mercier [Onera DADS, Châtillon], Fabrice Poirion [Onera DADS, Châtillon], Jean-Antoine Désidéri.

A novel algorithm for solving multiobjective 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 parallelizable. 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 [141].

6.12. Inverse Cauchy-Stokes problems solved as Nash games

Participants: Abderrahmane Habbal, Marwa Ouni [PhD, LAMSIN, Univ. Tunis Al Manar], Moez Kallel [LAMSIN, Univ. Tunis Al Manar].

We extend in two directions our results published in [30] to tackle ill posed Cauchy-Stokes inverse problems as Nash games. First, we consider the problem of detecting unknown pointwise sources in a stationary viscous fluid, using partial boundary measurements. The considered fluid obeys a steady Stokes regime, 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 source identification for the Cauchy-Stokes problem is ill-posed for both the sources and missing data reconstructions, and designing stable and efficient algorithms is challenging. We reformulate the problem as a three-player Nash game. Thanks to a source identifiability result derived for the Cauchy-Stokes 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 detection of the number, location and magnitude of the unknown sources. We provided the third player with the location and magnitude parameters as strategy, with a cost functional of Kohn-Vogelius type. In particular, the location is obtained through the computation of the topological sensitivity of the latter function. We propose an original algorithm, which we implemented using Freefem++. We present 2D numerical experiments for many different test-cases.The obtained results corroborate the efficiency of our 3-player Nash game approach to solve parameter or shape identification for Cauchy-Stokes problems.

The second direction is dedicated to the solution of the data completion problem for non-linear flows. We consider two kinds of non linearities leading to either a non newtonian Stokes flow or to Navier-Stokes equations. Our recent numerical results show that it is possible to perform a one-shot approach using Nash games : players exchange their respective state information and solve linear systems. At convergence to a Nash equilibrium, the states converge to the solution of the non linear systems. To the best of our knowledge, this is the first time such an approach is applied to solve Inverse problems for nonlinear systems.

6.13. Virtual FFR quantified with a generalized flow model using Windkessel boundary conditions ; Application to a patient-specific coronary tree

Participants: Abderrahmane Habbal, Keltoum Chahour [PhD, ACUMES and EMI, Univ. Mohammed V], Rajae Aboulaich [EMI, Univ. Mohammed V], Nejib Zemzemi [Inria Bordeaux, EPI CARMEN], Mickaël Binois.

Fractional flow reserve (FFR) has proved its efficiency in improving patients diagnosis. From both economical and clinical viewpoints, a realistic simulation of vascular blood flow inside the coronary arteries could be a better alternative to the invasive FFR. In this view, we consider a 2D reconstructed left coronary tree with two artificial lesions of different degrees. We use a generalized fluid model with a Carreau law and use a coupled multidomain method to implement Windkessel boundary conditions at the outlets. We introduce our methodology to quantify the virtual FFR, and lead several numerical experiments. We compare FFR results from Navier Stokes versus generalized flow model, and for Windkessel versus traction free outlets boundary conditions or mixed outlets boundary conditions. We also investigate some sources of uncertainty that the FFR index might encounter during the invasive procedure, in particular the arbitrary position of the distal sensor. The computational FFR results show that the degree of stenosis is not enough to classify a lesion, while there is a good agreement between Navier Stokes and the non Newtonian flow model adopted in classifying coronary lesions. Furthermore, we highlight that the lack of standardization while making FFR measurement might be misleading regarding the significance of stenosis [76].

CAGIRE Project-Team

7. New Results

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

Participant: Pascal Bruel.

The latest version of the pressure-correction algorithm developed in the last years in close partnership with Prof. E. Dick (Ghent University, Belgium) and Dr. Y. Moguen (UPPA, France) has been published this year [14]. Beyond its promotion [25], future efforts will be directed towards its extension to reacting single phase flows.

7.2. Simulation of a jet in a supersonic cross-flow

Participant: Pascal Bruel.

In our joint work, published this year with our Kazakh colleagues [10], we have focused on detailing the vortical patterns present in the structure of a sonic jet injected normally into a supersonic crossflow. Such a generic flow configuration is considered to feature some prominent characteristics encountered in propulsion system based on supersonic combustion (scramjet). A critical pressure ratio value beyond which new vortical structures are appearing has been evidenced. Contacts have been taken with ONERA to have access to their experimental database which is much more developed than the one we had access to so far. Some specific adaptation will have to be conducted though, in order to adapt the simulation to the slightly different flow configuration considered by ONERA.

7.3. Experiments and simulations related to flows over aerial tanks

Participant: Pascal Bruel.

These results have been obtained in the framework of the cooperation with the National University of Córdoba (Argentina).

- Predicting the pressure loads produced by the atmospheric wind flow over a cylindrical vertical tank

  Pressure distributions obtained using different RANS turbulence models were compared with experimental data obtained in wind tunnel tests for a tank with a closed roof. We have considered a flat shape and a conical roof of 25 degrees. Combinations of aspect ratios equal to 0.5, 1 and 2, and Reynolds numbers equal to 250000, 290000 and 340000 were simulated. The results of the numerical model were compared with those obtained in experimental tests in a wind tunnel of the atmospheric boundary layer using a rigid tank model. We have worked to obtain a stable atmospheric boundary layer in the complete domain using the correct boundary conditions for the implemented RANS models. After that, we have developed numerical simulations for the flow around the tanks inside the atmospheric boundary layer. These results have been published in [17].

- Studying the interaction of a wall with the flow around two cylinders arranged in tandem

For this configuration, the cylinders were immersed in a flow with a boundary layer profile at a subcritical Reynolds number (Re=10000). The three-dimensional transient turbulent flow around the cylinders was simulated numerically using the SAS turbulence model. The effects of wake interference due to both the proximity between the cylinders and their position with respect to the wall were examined through the values of drag, lift and pressure coefficients. The details of the flow fields in the near wake of the cylinders were also studied. The results were compared with experimental and numerical results reported in the literature, and with the case of a single cylinder near a wall. These results have been published in [15]. In parallel, a specific test section for the team's Maveric test facility has been developed. It gives the possibility to accommodate wall mounted cylinder(s) that represent a scaled down version of real horizontal tanks. The objective here is to generate validation data. Particle image velocimetry (PIV) measurements have been carried out during the 1-month stay of Mauro Grioni in Pau in September 2019.

- Simulating the effects of explosions on liquid fuel storage tanks.

  The fast release of energy in explosive processes produces intense shock waves (blast waves). The interaction of these waves with obstacles such as tanks can be extremely destructive. As a first step towards the full simulation of a blast wave with a tank, we have studied the capabilities of OpenFOAM to simulate a blast wave. The numerical results were compared in a cylindrical configuration with the analytical solution provided by the Sedov theory. A special attention has been paid to evaluate the influence of the reconstruction functions in the Euler flux (Kurganov scheme) on the numerical results. The predicted position and velocity of the generated shock wave as well as the pressure jump and its evolution behind the shock were in good agreement with their theoretical counterparts. These results have been published in [16].

7.4. A density-based numerical flux for high order simulation of low Mach flows with acoustics

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. These results have been published in [12].

7.5. Conjugate heat transfer with different fluid-solid physical properties: a new elliptic blending second-moment closure

Participants: Rémi Manceau, Gaëtan Mangeon.

Our approach to model the wall/turbulence interaction, based on Elliptic Blending, was successfully applied to flows with standard thermal boundary conditions at the walls [11]. However, Conjugate Heat Transfer, which couples fluid and solid domains, are particularly challenging for turbulence models. We have developed an innovative model, the Elliptic Blending Differential Flux Model, to account for the influence of various wall thermal boundary conditions on the turbulent heat flux and the temperature variance. An assessment of this new model in Conjugate Heat Transfer has been performed for several values of fluid-solid thermal diffusivity and conductivity ratios. A careful attention is paid to the discontinuity of the dissipation rate associated with the temperature variance at the fluid-solid interface. The analysis is supported by successful comparisons with Direct Numerical Simulations [30].

7.6. Eddy-viscosity models sensitized to buoyancy effects for predicting natural convection flows

Participants: Rémi Manceau, Saad Jameel.

Eddy-viscosity turbulence models have been sensitized to the effects of buoyancy, in order to improve the prediction in natural convection flows. The approach extends in a linear way the constitutive relations for the Reynolds stress and the turbulent heat flux, in order to account for the anisotropic influence of buoyancy. The novelty of this work involves the buoyancy extension applied to two very different eddy-viscosity models, which leads to encouraging results for the highly challenging case of the differentially heated vertical channel [27], [22].

7.7. Development and validation of an improved HTLES approach

Participants: Rémi Manceau, Vladimir Duffal, Hassan Afailal, Franck Mastrippolito, Pascal Bruel.

The HTLES (hybrid temporal LES) approach, developed by the team, has been improved by introducing shielding functions and an internal consistency constraint to enforce the RANS behavior in the near-wall regions [18]. The influence of the underlying closure model was studied by applying HTLES to two RANS models: the k-ω SST and the BL-v2/k. The validation, carried out using two different solvers, Code_Saturne (collaboration with EDF) and Converge-CFD (collaboration with IFPEN), encompassed different type of internal flows: channel, periodic hill, internal combustion engines (in fixed position and with a moving piston), jet in crossflow [21], [9]. The robustness of HTLES to grid coarsening and the accuracy of the predictions at a reduced numerical cost compared to LES was demonstrated. Notably, the capacity of HTLES to provide information on velocity and pressure temporal fluctuations at the wall was assessed, offering a cost-saving alternative to LES to predict unsteady loads. One of the major limitation of HTLES, i.e., the fact that it is based on statistically averaged quantities, which are challenging to estimate in non-stationary flows, has been removed, by approximating the statistical average by a Dynamic Temporal Filter.

7.8. Compact WENO, positivity preserving stabilization of discontinuous Galerkin methods

Participant: Vincent Perrier.

Jointly with Alireza Mazaheri (NASA Langley) and Chi Wang Shu, we have developed a compact WENO stabilization that moreover ensures the positivity of physical quantities. The work was published in [13].

CARDAMOM Project-Team

7. New Results

7.1. Modelling of free surface flows

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

  This year we continued our work on free surface flow modelling. We can dived our work on four main axis. First, we presented a depth-integrated Boussinesq model for the efficient simulation of nonlinear wave-body interaction [4]. The model exploits a ÂÂunifiedÂÂ Boussinesq framework, i.e. the fluid under the body is also treated with the depth-integrated approach. The unified Boussinesq approach was initially proposed by Jiang [60] and recently analysed by Lannes [67]. The choice of Boussinesq-type equations removes the vertical dimension of the problem, resulting in a wave-body model with adequate precision for weakly nonlinear and dispersive waves expressed in horizontal dimensions only. The framework involves the coupling of two different domains with different flow characteristics. Inside each domain, the continuous spectral/hp element method is used to solve the appropriate flow model since it allows to achieve high-order, possibly exponential, convergence for non-breaking waves. Flux-based conditions for the domain coupling are used, following the recipes provided by the discontinuous Galerkin framework. The main contribution of this work is the inclusion of floating surface-piercing bodies in the conventional depth-integrated Boussinesq framework and the use of a spectral/hp element method for high-order accurate numerical discretization in space. The model is verified using manufactured solutions and validated against published results for wave-body interaction. The model is shown to have excellent accuracy and is relevant for applications of waves interacting with wave energy devices. The outcome of this work is the phd thesis of Uberto Bosi.[1].

  Second, a detailed analysis of undular bore dynamics in channels of variable cross-section is performed and presented in [5] . Two undular bore regimes, low Froude number (LFN) and high Froude number (HFN), are simulated with a Serre Green Naghdi model, and the results are compared with the experiments by Treske (1994). We show that contrary to Favre waves and HFN bores, which are controlled by dispersive non-hydrostatic mechanisms, LFN bores correspond to a hydrostatic phenomenon. The dispersive-like properties of the LFN bores is related to wave refraction on the banks in a way similar to that of edge waves in the near shore. A fully hydrostatic asymptotic model for these dispersive-like bores is derived and compared to the observations, confirming our claim.

  An other part of our last year's work was focused on wave breaking for Boussineq-type equations [3]. The aim of this work was to develop a model able to represent the propagation and transformation of waves in nearshore areas. The focus is on the phenomena of wave breaking, shoaling and run-up. These different phenomena are represented through a hybrid approach obtained by the coupling of non-linear Shallow Water equations with the extended Boussinesq equations of Madsen and Sorensen. The novelty is the switch tool between the two modelling equations: a critical free surface Froude criterion. This is based on a physically meaningful new approach to detect wave breaking, which corresponds to the steepening of the wave's crest which turns into a roller. To allow for an appropriate discretization of both types of equations, we consider a finite element Upwind Petrov Galerkin method with a novel limiting strategy, that guarantees the preservation of smooth waves as well as the monotonicity of the results in presence of discontinuities.We provide a detailed discussion of the implementation of the newly proposed detection method, as well as of two other well known criteria which are used for comparison. An extensive benchmarking on several problems involving different wave phenomena and breaking conditions allows to show the robustness of the numerical method proposed, as well as to assess the advantages and limitations of the different detection methods.

We also continue to work on the modelling of free surface flows by investigating a new family of models, derived from the so-called Isobe-Kakinuma models. The Isobe–Kakinuma model is a system of Euler–Lagrange equations for a Lagrangian approximating Luke's Lagrangian for water waves. In [23], We consider the Isobe–Kakinuma model for two-dimensional water waves in the case of the flat bottom. We show theoretically the existence of a family of small amplitude solitary wave solutions to the Isobe–Kakinuma model in the long wave regime. We have also performed numerical computations for a toy system included large amplitude solitary wave solutions. Our computations suggest the existence of a solitary wave of extreme form with a sharp crest. This models seems very promising for future research.

7.2. Modelling of icing and de-icing of aircrafts

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

  In-flight icing on an aircrafts surface can be a major hazard in aeronautics's safety. Numerical simulations of ice accretion on aircraft is a common procedure to anticipate ice formation when flying in a supercooled water droplets cloud. Numerical simulations bring a better understanding of ice accretion phenomena, performance degradations and lead to even more efficient thermal de-icing systems designs. Such simulations imply modelling the phase change of water and the mass and energy transfers. The Messinger model developed in the 1950 is still used today as a reliable basis for new models development. This model estimates the ice growth rate using mass and energy balances coupled to a runback water flow. The main parameter introduced with this approach is the freezing fraction, denoting the fraction of incoming water that effectively freezes on the airfoil.

  In-flight ice accretion code predictions depend on heat loss over rough surfaces. The equivalent sand grain roughness models the friction coefficient, but an additional model is needed for heat transfer prediction. The turbulent Prandtl number correction and the sublayer Stanton-based models are commonly used. This year, both models have been used with the Spalart-Allmaras turbulence model to predict heat transfer over rough surfaces typical of ice accretion. The objective here is to compare the results of the two models. First, the sublayer Stanton-based model is rewritten in the context of a turbulent Prandtl number correction formulation. Then, the two models are implemented in the open source software, SU2, and then verified and validated for flow over rough flat plates, airfoils, and wings. The two models' predictions evolve differently with the local Reynolds number, but are always within the experimental 20% error margin. The paper related to those developments are under revision.

  In the work [17], the objective is to model an ice accretion on an airfoil using a Messinger-based approach and to make a sensitivity analysis of roughness models on the ice shape. The test case is performed on a 2D NACA0012 airfoil. A typical test case on a NACA0012 airfoil under icing conditions is run and confronted with the literature for verification prior to further investigations. Ice blocks profiles comparisons will highlight the differences implied by the choice of the roughness correction, which impact the heat transfer coefficient.

  Numerical simulation of separated flow around an iced airfoil is still a challenge. Predictions of post-stall aerodynamic performance by RANS models are unsatisfactory. Recent hybrid RANS/LES methods, based on modified DDES models, have shown promising results for separated flow. However, questions still arise about the best compromise between computation time and accuracy for the unsteady 3D simulations. The span width of the domain and the best grid practice to obtain accurate results still has to be investigated, especially taking into account the recent method improvements. A recent method such as shear-layer adapted DDES should give acceptable flow prediction with a relatively coarse mesh. In the paper [18], we further study the effects of span width length on predicted aerodynamic coefficients and on the pressure coefficient. The study is done using the open-source software SU2. The backward facing step and a stalled NACA0012 is used to validate the numerical results. Then, the numerical flow around an iced Model 5-6 is studied, especially the flow within the separation bubble behind the ice. The accuracy of the CFD results is discussed and a recommendation is made about the span width of the computation domain and the grid size.

In order to spare time and resources while increasing the results' accuracy of the stalled wing configuration's aerodynamic coefficients, the following study [16] offers a parametric grid study for the DDES model. For three different grid refinements, characteristics of lift and eddy phenomena are presented and compared to determine, for an infinite wing, the best compromise between time and resources' consumption, and results's accuracy. Using the open software SU2 6.1 (Stanford University Unstructured), we generate three different types of grid refinements around an airfoil, developed spanwise to obtain a straight wing. On the same stalled configuration for each mesh, CFD solutions are ran with the DDES model, and the raw data are post processed with the open software ParaView 5.6. We then compare the aerodynamic coefficients' distributions obtained by the three mesh. The general modelling of vortex shedding's topology and turbulence viscosity are compared with the literature to ensure the right rendering of vortex structures. Chordwise pressure and friction coefficients' distributions as well as the spanwiselift coefficient are also compared. We conclude with the optimum mesh in term of results and resources' consumption.

7.3. High order embedded and immersed boundary methods

- Participants: Héloïse Beaugendre, Mirco Ciallella, Benjamin Constant and Mario Ricchiuto
- Corresponding member: Héloïse Beaugendre
  In the last years the team has invested some effort in developing the high order embedded method known as "shifted boundary method". In this method, geometrical boundaries are not meshed exactly but embedded in the mesh. Boundary conditions are imposed on a surrogate boundary, toughly defined by the collection of mesh faces "closest" to the true boundary. To recover high order of accuracy, the boundary condition imposed on this surrogate boundary is modified to account for the distance from the true boundary.

  This year's work has focused on two aspects. First, we proposed an efficient extension of the method to elliptic diffusion equations in mixed form (e.g., Darcy flow, heat diffusion problems with rough coefficients, etc.) [10] Our aim is to obtain an improved formulation that, for linear finite elements, is at least second-order accurate for both flux and primary variable, when either Dirichlet or Neumann boundary conditions are applied. Following previous work of Nishikawa and Mazaheri in the context of residual distribution methods, we consider the mixed form of the diffusion equation (i.e., with Darcy-type operators), and introduce an enrichment of the primary variable. This enrichment is obtained exploiting the relation between the primary variable and the flux variable, which is explicitly available at nodes in the mixed formulation. The proposed enrichment mimics a formally quadratic pressure approximation, although only nodal unknowns are stored, similar to a linear finite element approximation. We consider both continuous and discontinuous finite element approximations and present two approaches: a non-symmetric enrichment, which, as in the original references, only improves the consistency of the overall method; and a symmetric enrichment, which enables a full error analysis in the classical finite element context. Combined with the shifted boundary method, these two approaches are extended to high-order embedded computations, and enable the approximation of both primary and flux (gradient) variables with second-order accuracy, independently on the type of boundary conditions applied. We also show that the the primary variable is third-order accurate, when pure Dirichlet boundary conditions are embedded.

  Second, using the same ideas underlying the shifted boundary method, a novel approach to handle shock waves has been proposed. In this method shocks are seen as embedded boundaries on which appropriately shifted jump conditions are imposed, allowing to connect the upstream and downstream domains. This new technique, named "shifted shock-fitting", has been implemented on two-dimensional unstructured grids to deal with shocks by treating them as they were immersed boundary. The new algorithm is aimed at coupling a floating shock-fitting technique with the shifted

boundary method, so far introduced only to simulate flows with embedded boundaries (see [15], full length paper in revision on *J.Comput.Phys.*).
A new PhD in collaboration with ONERA has started (Benjamin Constant 's thesis) involving the numerical simulation of unsteady flows around complex geometries in aeronautics. In the CFD simulation process, mesh generation is the main bottleneck when one wishes to study realistic configurations, such as an aircraft landing gear. A mesh can represent a month to several months of engineer time for a specialist, which is prohibitive in the pre-design phase where several geometries are evaluated in a very short time frame. For this reason, Inria and Onera have been interested for several years in the development of an immersed boundary method, which does not require representing obstacles by mesh conforming to the wall, thus simplifying the generation of mesh. The consideration of the wall is carried out by the introduction of a forcing term at certain points in the vicinity of obstacles. In our approach, this technique is combined with a method of generating adaptive octree cartesian mesh. This allows us to exploit the advantages of Cartesian mesh (generation and rapid adaptation, performance gains of a dedicated Cartesian solver). In order to model the boundary layer, a wall model is used to avoid an extra cost. This method has been implemented for the simulation of steady turbulent flows around geometries studied in compressible aerodynamics (winged fuselage, engine air intake, helicopter fuselage...), providing a very good compromise between the quality of the aerodynamic solution and the time it takes to return the solution from the definition of geometry. However, the quality of the solution obtained by steady simulations is not sufficient to predict the acoustics satisfactorily. Indeed, oscillations appear for certain sizes of interest (such as turbulent viscosity or pressure fluctuations) in the vicinity of the wall. In addition, the passage of grids of different levels causes reflections, which can greatly degrade the prediction of the acoustic solution. The objective of this thesis is to solve these two problems in order to be able to perform unsteady simulations around complex geometries, such as a landing gear. On the one hand, we will study an algorithm to regularize the solution at the points of interest of the IBM method located near the wall. Together, we will also be interested in improving the wall model, in collaboration with modeling specialists from the department. We will do a study by error estimators to analyze the impact of these improvements on the solution. Validations on academic test cases will be carried out. A second step is to improve the transfer of the solution between grids of different levels (for which the mesh size double). We will propose an algorithm to regularize this passage, by geometrically modifying the mesh and by modifying the transfer formula of the solution at the passage of the fitting. A validation will be carried out on an unsteady case of LEISA profile. Finally, a demonstrative application that is both geometrically complex and of acoustic interest will be performed, typically a LAGOON or Gulfstream landing gear.

7.4. Composites Materials

- Participants: Giulia Bellezza, Mathieu Colin and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto
  Self-healing is an important phenomenon in new-generation refractory ceramic-matrix composites, obtained by the oxidation of a glass-forming phase in the composite. The dynamics of oxygen diffusion, glass formation and flow are the basic ingredients of a self-healing model that has been developed here in 2D in a trans-verse crack of a mini composite [11]. The presented model can work on a realistic image of the material section and is able to simulate healing and quantify the exposure of the material to oxygen, a prerequisite for its lifetime prediction. Crack reopening events are handled satisfactorily, and secondary healing can be simulated. This papers describes and discusses a typical case in order to show the model potentialities.

  Additional work involve two main topics. The first one is dedicated to the modeling of the propagation of a self-healing oxyde in a crack. The aim here is to introduce new models which describe both the self-healing behavior and oxygen diffusion towards fibers. In general, the evolution of an incompressible fluid can be described by the Navier-Stokes equations. However, we observe that a direct numerical method applied to these equations will induce a significant computational cost, especially in our case, due to the long lifespan of the material. Thus, alternatively, we derive several asymptotic models obtained by performing a dimensional analysis on the Navier-Stokes equations : we focus here on shallow water models and thin film models. The second aspect under study is more theoretical. 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.

7.5. Adaptation techniques

- Participants: Nicolas Barral, Héloïse Beaugendre, Luca Cirrottola, Algiane Froehly, Mario Ricchiuto.
- Corresponding member: Nicolas Barral
  In [14] we presented an algorithm to perform PDE-based r-adaptation in three-dimensional numerical simulations of unsteady compressible flows on unstructured meshes. A Laplacian-based model for the moving mesh is used to follow the evolving shock-wave patterns in the fluid flow, while the finite volume ALE formulation of the flow solver is employed to implicitly perform a conservative re-mapping of the solution from the previous to the current mesh, at each time step of the simulation.We show the application of this method to compressible flows on three-dimensional geometries. To this aim, an improved relaxation scheme has been developed in order to preserve the validity of the mesh throughout the time simulation in three dimensions, where the geometrical constraints typically restrict the allowable mesh motion.

  Similar adaptive strategies have been investigate for shallow water flows in the context of space-time residual distribution methods [7]. In the scalar case, these schemes can be designed to be unconditionally (w.r.t. the time step) positive, even on the distorted space-time prisms which arise from moving the nodes of an unstructured triangular mesh. Consequently, a local increase in mesh resolution does not impose a more restrictive stability constraint on the time-step, which can instead be chosen according to accuracy or physical requirements. Moreover, schemes of this type are analogous to conservative ALE formulations and automatically satisfy a discrete geometric conservation law. For shallow water flows over variable bed topography, the so-called C-property (retention of hydrostatic balance between flux and source terms, required to maintain the steady state of still, flat, water) can also be satisfied by considering the mass balance equation in terms of free surface level instead of water depth, even when the mesh is moved. Combined with a simple implementation of Laplacian based r-adaptation, this technique has been shown to allow up to 60% CPU time savings for a given error.

  We also extended these methods to curvilinear coordinates to do shallow water simulations on the sphere for oceanographic applications [2]. To provide enhanced resolution of moving fronts present in the flow we consider adaptive discrete approximations on moving triangulations of the sphere. To this end, we re- state all Arbitrary Lagrangian Eulerian (ALE) transport formulas, as well as the volume transformation laws, for a 2D manifold. Using these results, we write the set of ALE-SWEs on the sphere. We then propose a Residual Distribution discrete approximation of the governing equations. Classical properties as the DGCL and the C-property (well balancedness) are reformulated in this more general context. An adaptive mesh movement strategy is proposed. The discrete framework obtained is thoroughly tested on standard benchmarks in large scale oceanography to prove their potential as well as the advantage brought by the adaptive mesh movement.

DEFI Project-Team

5. New Results

5.1. Qualitative and quantitative methods for inverse problems

5.1.1. Differential tomography of micromechanical evolution in elastic materials of unknown micro/macrostructure

H. haddar and F. Pourahmadian

Differential evolution indicators are introduced for 3D spatiotemporal imaging of micromechanical processes in complex materials where progressive variations due to manufacturing and/or aging are housed in a highly scattering background of a-priori unknown or uncertain structure. In this vein, a three-tier imaging platform is established where: (1) the domain is periodically (or continuously) subject to illumination and sensing in an arbitrary configuration; (2) sequential sets of measured data are deployed to distill segment-wise scattering signatures of the domain's internal structure through carefully constructed, non-iterative solutions to the scattering equation; and (3) the resulting solution sequence is then used to rigorously construct an imaging functional carrying appropriate invariance with respect to the unknown stationary components of the background e.g., pre-existing interstitial boundaries and bubbles. This gives birth to differential indicators that specifically recover the 3D support of micromechanical evolution within a network of unknown scatterers. The direct scattering problem is formulated in the frequency domain where the background is comprised of a random distribution of monolithic fragments. The constituents are connected via highly heterogeneous interfaces of unknown elasticity and dissipation which are subject to spatiotemporal evolution. The support of internal boundaries are sequentially illuminated by a set of incident waves and thusinduced scattered fields are captured over a generic observation surface. The performance of the proposed imaging indicator is illustrated through a set of numerical experiments for spatiotemporal reconstruction of progressive damage zones featuring randomly distributed cracks and bubbles [35].

5.1.2. Microwave tomographic imaging of cerebrovascular accidents by using high-performance computing

P.-H. Tournier, I. Aliferis, M. Bonazzoli, M. De Buhan, M. Darbas, V. Dolean, F. Hecht, P. Jolivet, I. El Kanfoud, C. Migliaccio, F. Nataf, C. Pichot, S. Semenov

The motivation of this work is the detection of cerebrovascular accidents by microwave tomographic imaging. This requires the solution of an inverse problem relying on a minimization algorithm (for example, gradient-based), where successive iterations consist in repeated solutions of a direct problem. The reconstruction algorithm is extremely computationally intensive and makes use of efficient parallel algorithms and high-performance computing. The feasibility of this type of imaging is conditioned on one hand by an accurate reconstruction of the material properties of the propagation medium and on the other hand by a considerable reduction in simulation time. Fulfilling these two requirements will enable a very rapid and accurate diagnosis. From the mathematical and numerical point of view, this means solving Maxwell's equations in time-harmonic regime by appropriate domain decomposition methods, which are naturally adapted to parallel architectures [20].

5.1.3. A Factorization Method for Inverse Time Domain Obstacles with Impedance Boundary Conditions

H. Haddar and X. Liu

We develop a factorization method to obtain explicit characterization of a (possibly non-convex) impedance 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 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. We provide validating numerical examples in 2D on synthetic data. The latter is generated using a FDTD solver with PML. An article on this topic is under preparation.

5.1.4. 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 [2].

5.1.5. Factorization Method for Imaging a Local Perturbation in Inhomogeneous Periodic Layers from Far Field Measurements

H. Haddar and A. Konschin

We analyze the Factorization method to reconstruct the geometry of a local defect in a periodic absorbing layer using almost only incident plane waves at a fixed frequency. A crucial part of our analysis relies on the consideration of the range of a carefully designed far field operator, which characterizes the geometry of the defect. We further provide some validating numerical results in a two dimensional setting [9].

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

L. Audibert, H. Girardon and H. Haddar

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 experimentation with synthetic data demonstrated the viability of our approach. The approach is also successfully validated against experimental data. An article on this topic is under preparation.

5.1.7. On quasi-reversibility solutions to the Cauchy problem for the Laplace equation: regularity and error estimates

L. Bourgeois, L. Chesnel

We are interested in the classical ill-posed Cauchy problem for the Laplace equation. One method to approximate the solution associated with compatible data consists in considering a family of regularized well-posed problems depending on a small parameter $\varepsilon > 0$. In this context, in order to prove convergence of finite elements methods, it is necessary to get regularity results of the solutions to these regularized problems which hold uniformly in ε. In the present work, we obtain these results in smooth domains and in 2D polygonal geometries. In presence of corners, due the particular structure of the regularized problems, classical techniques *à la* Grisvard do not work and instead, we apply the Kondratiev approach. We describe the procedure in detail to keep track of the dependence in ε in all the estimates. The main originality of this study lies in the fact that the limit problem is ill-posed in any framework [4].

5.1.8. Data Completion Method For the Helmholtz Equation Via Surface Potentials for Partial Cauchy Data

M. Aussal, Y. Boukari and H. Haddar

We propose and study a data completion algorithm for recovering missing data from the knowledge of Cauchy data on parts of the same boundary. The algorithm is based on surface representation of the solution and is presented for the Helmholtz equation. This work is an extension of the data completion algorithm proposed by the two last authors where the case of data available of a closed boundary was studied. The proposed method is a direct inversion method robust with respect to noisy incompatible data. Classical regularization methods with discrepancy selection principles can be employed and automatically lead to a convergent schemes as the noise level goes to zero. We conduct 3D numerical investigations to validate our method on various synthetic examples [31].

5.2. Invisiblity and transmission eigenvalues

5.2.1. Inside-outside duality with artificial backgrounds

L. Audibert, L. Chesnel, H. Haddar

We use the inside-outside duality approach proposed by Kirsch-Lechleiter to identify transmission eigenvalues associated with artificial backgrounds. We prove that for well chosen artificial backgrounds, in particular for the ones with zero index of refraction at the inclusion location, one obtains a necessary and sufficient condition characterizing transmission eigenvalues via the spectrum of the modified far field operator. We also complement the existing literature with a convergence result for the invisible generalized incident field associated with the transmission eigenvalues [1].

5.2.2. Surface waves in a channel with thin tunnels and wells at the bottom: non-reflecting underwater topography

L. Chesnel, S.A. Nazarov, J. Taskinen

We consider the propagation of surface water waves in a straight planar channel perturbed at the bottom by several thin curved tunnels and wells. We propose a method to construct non reflecting underwater topographies of this type at an arbitrary prescribed wave number. To proceed, we compute asymptotic expansions of the diffraction solutions with respect to the small parameter of the geometry taking into account the existence of boundary layer phenomena. We establish error estimates to validate the expansions using advances techniques of weighted spaces with detached asymptotics. In the process, we show the absence of trapped surface waves for perturbations small enough. This analysis furnishes asymptotic formulas for the scattering matrix and we use them to determine underwater topographies which are non-reflecting. Theoretical and numerical examples are given [6]

5.2.3. Exact zero transmission during the Fano resonance phenomenon in non symmetric waveguides

L. Chesnel, S.A. Nazarov

We investigate a time-harmonic wave problem in a waveguide. We work at low frequency so that only one mode can propagate. It is known that the scattering matrix exhibits a rapid variation for real frequencies in a vicinity of a complex resonance located close to the real axis. This is the so-called Fano resonance phenomenon. And when the geometry presents certain properties of symmetry, there are two different real frequencies such that we have either $R = 0$ or $T = 0$, where R and T denote the reflection and transmission coefficients. In this work, we prove that without the assumption of symmetry of the geometry, quite surprisingly, there is always one real frequency for which we have $T = 0$. In this situation, all the energy sent in the waveguide is backscattered. However in general, we do not have $R = 0$ in the process. We provide numerical results to illustrate our theorems [33].

5.2.4. Homogenization of Maxwell's equations and related scalar problems with sign-changing coefficients

R. Bunoiu, L. Chesnel, K. Ramdani, M. Rihani

In this work, we are interested in the homogenization of time-harmonic Maxwell's equations in a composite medium with periodically distributed small inclusions of a negative material. Here a negative material is a material modelled by negative permittivity and permeability. Due to the sign-changing coefficients in the equations, it is not straightforward to obtain uniform energy estimates to apply the usual homogenization techniques. The goal of this work is to explain how to proceed in this context. The analysis of Maxwell's equations is based on a precise study of two associated scalar problems: one involving the sign-changing permittivity with Dirichlet boundary conditions, another involving the sign-changing permeability with Neumann boundary conditions. For both problems, we obtain a criterion on the physical parameters ensuring uniform invertibility of the corresponding operators as the size of the inclusions tends to zero. In the process, we explain the link existing with the so-called Neumann-Poincaré operator, complementing the existing literature on this topic. Then we use the results obtained for the scalar problems to derive uniform energy estimates for Maxwell's system. At this stage, an additional difficulty comes from the fact that Maxwell's equations are also sign-indefinite due to the term involving the frequency. To cope with it, we establish some sort of uniform compactness result [32].

5.3. Shape and topology optimization

5.3.1. Null space gradient flows for constrained optimization with applications to shape optimization

G. Allaire, F. Feppon and C. Dapogny

The purpose of this article is to introduce a gradient-flow algorithm for solving equality and inequality constrained optimization problems, which is particularly suited for shape optimization applications. We rely on a variant of the Ordinary Differential Equation (ODE) approach proposed by Yamashita for equality constrained problems: the search direction is a combination of a null space step and a range space step, aiming to decrease the value of the minimized objective function and the violation of the constraints, respectively. Our first contribution is to propose an extension of this ODE approach to optimization problems featuring both equality and inequality constraints. In the literature, a common practice consists in reducing inequality constraints to equality constraints by the introduction of additional slack variables. Here, we rather solve their local combinatorial character by computing the projection of the gradient of the objective function onto the cone of feasible directions. This is achieved by solving a dual quadratic programming subproblem whose size equals the number of active or violated constraints. The solution to this problem allows to identify the inequality constraints to which the optimization trajectory should remain tangent. Our second contribution is a formulation of our gradient flow in the context of—infinite-dimensional—Hilbert spaces, and of even more general optimization sets such as sets of shapes, as it occurs in shape optimization within the framework of Hadamard's boundary variation method. The cornerstone of this formulation is the classical operation of extension and regularization of shape derivatives. The numerical efficiency and ease of implementation of our algorithm are demonstrated on realistic shape optimization problems. An article on this topic is under preparation.

5.3.2. A variational formulation for computing shape derivatives of geometric constraints along rays

G. Allaire, F. Feppon and C. Dapogny

In the formulation of shape optimization problems, multiple geometric constraint functionals involve the signed distance function to the optimized shape Ω. The numerical evaluation of their shape derivatives requires to integrate some quantities along the normal rays to Ω, a task that is usually achieved thanks to the method of characteristics. The goal of the present paper is to propose an alternative, variational approach for this purpose. Our method amounts, in full generality, to compute integral quantities along the characteristic curves of a given velocity field without requiring the explicit knowledge of these curves on the spatial discretization; it rather relies on a variational problem which can be solved conveniently by the finite element method. The well-posedness of this problem is established thanks to a detailed analysis of weighted graph spaces of the advection operator $\beta \cdot \nabla$ associated to a $\mathcal{C}^1$ velocity fields β. One novelty of our approach is the ability to handle velocity fields with possibly unbounded divergence: we do not assume $\div(\beta) \in L^\infty$. Our working assumptions are fulfilled in the context of shape optimization of $\mathcal{C}^2$ domains Ω, where the velocity field $\beta = \nabla d_\Omega$ is an extension of the unit outward normal vector to the optimized shape. The efficiency of our variational method with respect to the direct integration of numerical quantities along rays is evaluated on several numerical examples. Classical albeit important implementation issues such as the calculation of a shape's curvature and the detection of its skeleton are discussed. Finally, we demonstrate the convenience and potential of our method when it comes to enforcing maximum and minimum thickness constraints in structural shape optimization. An article on this topic is under preparation.

5.3.3. 3-d topology optimization of modulated and oriented periodic microstructures by the homogenization method

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

This paper is motivated by the optimization of so-called lattice materials which are becoming increasingly popular in the context of additive manufacturing. Generalizing our previous work in 2-d we propose a method for topology optimization of structures made of periodically perforated material, where the microscopic periodic cell can be macroscopically modulated and oriented. This method is made of three steps. The first step amounts to compute the homogenized properties of an adequately chosen parametrized microstructure (here, a cubic lattice with varying bar thicknesses). The second step optimizes the homogenized formulation of the problem, which is a classical problem of parametric optimization. The third, and most delicate, step projects the optimal oriented microstructure at a desired length scale. Compared to the 2-d case where rotations are parametrized by a single angle, to which a conformality constraint can be applied, the 3-d case is more involved and requires new ingredients. In particular, the full rotation matrix is regularized (instead of just one angle in 2-d) and the projection map which deforms the square periodic lattice is computed component by component. Several numerical examples are presented for compliance minimization in 3-d. An article on this topic is under preparation.

5.4. Analysis of some wave problems

5.4.1. 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 prescribe 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. [5]

5.4.2. Domain decomposition preconditioning for the high-frequency time-harmonic Maxwell equations with absorption

M. Bonazzoli, V. Dolean, I. G. Graham, E. A. Spence and P.-H. Tournier

In this work we rigorously analyse preconditioners for the time-harmonic Maxwell equations with absorption, where the PDE is discretised using curl-conforming finite-element methods of fixed, arbitrary order and the preconditioner is constructed using additive Schwarz domain decomposition methods. The theory we developed shows that if the absorption is large enough, and if the subdomain and coarse mesh diameters and overlap are chosen appropriately, then the classical two-level overlapping additive Schwarz preconditioner (with PEC boundary conditions on the subdomains) performs optimally–in the sense that GMRES converges in a wavenumber-independent number of iterations–for the problem with absorption. An important feature of the theory is that it allows the coarse space to be built from low-order elements even if the PDE is discretised using high-order elements. It also shows that additive methods with minimal overlap can be robust. Several numerical experiments illustrate the theory and its dependence on various parameters. These experiments motivate some extensions of the preconditioners which have better robustness for problems with less absorption, including the propagative case. Finally, we illustrate the performance of these on two substantial applications; the first (a problem with absorption arising from medical imaging) shows the empirical robustness of the preconditioner against heterogeneity, and the second (scattering by a COBRA cavity) shows good scalability of the preconditioner with up to 3,000 processors [3].

5.4.3. Multi-Trace FEM-BEM formulation for acoustic scattering by composite objects

M. Bonazzoli, X. Claeys

This work is about the scattering of an acoustic wave by an object composed of piecewise homogenous parts and an arbitrarily heterogeneous part. We propose and analyze a formulation that couples, adopting a Costabel-type approach, boundary integral equations for the homogeneous subdomains with domain variational formulations for the heterogenous subdomain. This is an extension of Costabel FEM-BEM coupling to a multi-domain configuration, with junctions points allowed, i.e. points where three or more subdomains abut. Usually just the exterior unbounded subdomain is treated with the BEM; here we wish to exploit the BEM whenever it is applicable, that is for all the homogenous parts of the scattering object, since it yields a reduction in the number of unknowns compared to the FEM. Our formulation is based on the multi-trace formalism for acoustic scattering by piecewise homogeneous objects; here we allow the wavenumber to vary arbitrarily in a part of the domain. We prove that the bilinear form associated with the proposed formulation satisfies a Gårding coercivity inequality, which ensures stability of the variational problem if it is uniquely solvable. We identify conditions for injectivity and construct modified versions immune to spurious resonances. An article on this topic is under preparation.

5.4.4. Domain decomposition preconditioners for non-self-adjoint or indefinite problems

M. Bonazzoli, X. Claeys, F. Nataf, P.-H. Tournier

The matrices arising from the finite element discretization of problems such as high-frequency Helmholtz, time-harmonic Maxwell or convection-diffusion equations are not self-adjoint or positive definite. For this reason, it is difficult to analyze the convergence of Schwarz domain decomposition preconditioners applied to these problems. Note also that the conjugate gradient method cannot be used, and the analysis of the spectrum of the preconditioned matrix is not sufficient for methods suited for general matrices such as GMRES. In order to apply Elman-type estimates for the convergence of GMRES we need to prove an upper bound on the norm of the preconditioned matrix, and a lower bound on the distance of its field of values from the origin. We generalize the theory for the Helmholtz equation developed for the SORAS (Symmetrized Optimized Restricted Additive Schwarz) preconditioner, and we identify a list of assumptions and estimates that are sufficient to prove the two bounds needed for the convergence analysis for a general linear system. As an illustration of this technique, we prove estimates for the heterogenous reaction-convection-diffusion equation. An article on this topic is under preparation.

5.5. Diffusion MRI

J.-R. Li, K. V. Nguyen and T. N. Tran

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

We obtained the following results.

- The Bloch-Torrey partial differential equation can be used to describe 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 work proposes a finite element discretization on manifolds in order to efficiently simulate the diffusion MRI signal in domains that have a thin layer or a thin tube geometrical structure. The variable thickness of the three-dimensional domains is included in the weak formulation established on the manifolds. 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 agreements between the simulated signals using our proposed method and the reference signals for a wide range of diffusion MRI parameters. 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 [12].
- 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 the large cell neurons in the abdominal ganglia after creating geometrical configurations by segmenting high resolution T2-weighted (T2w) images to obtain the cell outline and then incorporating a manually generated nucleus. The results of the numerical simulations validate the claim that water diffusion in the large cell neurons is in the short diffusion time regime at 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, 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 [13].
- The complex transverse water proton magnetization subject to diffusion-encoding magnetic field

gradient pulses in a heterogeneous medium can be modeled by the multiple compartment Bloch-Torrey partial differential equation. Under the assumption of negligible water exchange between compartments, the time-dependent apparent diffusion coefficient can be directly computed from the solution of a diffusion equation subject to a time-dependent Neumann boundary condition. This work describes a publicly available MATLAB toolbox called SpinDoctor that can be used 1) to solve the Bloch-Torrey partial differential equation in order to simulate the diffusion magnetic resonance imaging signal; 2) to solve a diffusion partial differential equation to obtain directly the apparent diffusion coefficient; 3) to compare the simulated apparent diffusion coefficient with a short-time approximation formula. The partial differential equations are solved by $P1$ finite elements combined with built-in MATLAB routines for solving ordinary differential equations. The finite element mesh generation is performed using an external package called Tetgen. SpinDoctor provides built-in options of including 1) spherical cells with a nucleus; 2) cylindrical cells with a myelin layer; 3) an extra-cellular space enclosed either a) in a box or b) in a tight wrapping around the cells; 4) deformation of canonical cells by bending and twisting; 5) permeable membranes; Built-in diffusion-encoding pulse sequences include the Pulsed Gradient Spin Echo and the Oscillating Gradient Spin Echo. We describe in detail how to use the SpinDoctor toolbox. We validate SpinDoctor simulations using reference signals computed by the Matrix Formalism method. We compare the accuracy and computational time of SpinDoctor simulations with Monte-Carlo simulations and show significant speed-up of SpinDoctor over Monte-Carlo simulations in complex geometries. We also illustrate several extensions of SpinDoctor functionalities, including the incorporation of $T2$ relaxation, the simulation of non-standard diffusion-encoding sequences, as well as the use of externally generated geometrical meshes [10].

- The numerical simulation of the diffusion MRI signal arising from complex tissue micro-structures is helpful for understanding and interpreting imaging data as well as for designing and optimizing MRI sequences. The discretization of the Bloch-Torrey equation by finite elements is a more recently developed approach for this purpose, in contrast to random walk simulations, which has a longer history. While finite element discretization is more difficult to implement than random walk simulations, the approach benefits from a long history of theoretical and numerical developments by the mathematical and engineering communities. In particular, software packages for the automated solutions of partial differential equations using finite element discretization, such as FEniCS, are undergoing active support and development. However, because diffusion MRI simulation is a relatively new application area, there is still a gap between the simulation needs of the MRI community and the available tools provided by finite element software packages. In this paper, we address two potential difficulties in using FEniCS for diffusion MRI simulation. First, we simplified software installation by the use of FEniCS containers that are completely portable across multiple platforms. Second, we provide a portable simulation framework based on Python and whose code is open source. This simulation framework can be seamlessly integrated with cloud computing resources such as Google Colaboratory notebooks working on a web browser or with Google Cloud Platform with MPI parallelization. We show examples illustrating the accuracy, the computational times, and parallel computing capabilities. The framework contributes to reproducible science and open-source software in computational diffusion MRI with the hope that it will help to speed up method developments and stimulate research collaborations [11].
- 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 [34].
- We continued 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. An article on this topic is under preparation.

5.6. Uncertainty Quantification methods

5.6.1. Acceleration of Domain Decomposition Methods for Stochastic Elliptic Equations

João F. Reis, Olivier P. Le Maître, Pietro M. Congedo, Paul Mycek

We propose a Monte Carlo based method to compute statistics from a solution of a stochastic elliptic equation. Solutions are computed through an iterative solver. We present a parallel construction of a robust stochastic preconditioner to accelerate the iterative scheme. This preconditioner is built before the sampling, at an offline stage, based on a decomposition of the geometric domain. Once constructed, a realisation of the preconditioner is generated for each sample and applied to an iterative method to solve the corresponding deterministic linear system. This approach is not restricted to a single iterative method and can be adapted to different iterative techniques. We demonstrate the efficiency of this approach with extensive numerical results, divided into two examples. The first example is a one-dimensional equation. The reduced dimension of the first example allows the construction of global operators and consequently, an extensive analysis of the convergence and stability properties of the proposed approach. The second example is an analogous two-dimensional version. We demonstrate the performance of the proposed preconditioner by comparison with other deterministic preconditioners based on the median of the coefficient fields. An article on this topic is under preparation.

5.6.2. Clustering based design of experiments for Systems of Gaussian processes

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

Multi-physics problems in engineering can be often modeled using a System of Solvers (SoS), which is simply a set of solvers coupled together. SoS could be computationally expensive, for example in parametric studies, uncertainty quantification or sensitivity analysis, so typically requiring the construction of a global surrogate model of the SoS to perform such costly analysis. One recurrent strategy in literature consists of building a system of surrogate models where each solver is approximated with a local surrogate model. This approach can be efficient if good training sets for each surrogate can be generated, in particular on the intermediate variables (which are the outputs of an upstream solver and the inputs of a downstream one) that are a priori unknown. In this work, we propose a novel strategy to construct efficient training sets of the intermediate variables, using clustering-based techniques formulated for a systems of Gaussian processes (SoGP). In this way, improved coverage of the intermediate spaces is attained compared to randomly generated training sets. The performances of this approach are assessed on several test-cases showing that the clustering training strategy is systematically more efficient than randomly sampled training points [19].

5.6.3. Extension of AK-MCS for the efficient computation of very small failure probabilities

N. Razaaly, P.M. Congedo

We consider the problem of estimating a probability of failure p_f, defined as the volume of the excursion set of a complex (*e.g.* output of an expensive-to-run finite element model) scalar performance function J below a given threshold, under a probability measure that can be recast as a multivariate standard Gaussian law using an isoprobabilistic transformation. We propose a method able to deal with cases characterized by multiple failure regions, possibly very small failure probability p_f (say $\sim 10^{-6} - 10^{-9}$), and when the number of evaluations of J is limited. The present work is an extension of the popular Kriging-based active learning algorithm known as AK-MCS, permitting to deal with very low failure probabilities. The key idea merely consists in replacing the Monte-Carlo sampling, used in the original formulation to propose candidates and evaluate the failure probability, by a centered isotropic Gaussian sampling in the standard space, which standard deviation is iteratively tuned. This *extreme* AK-MCS (eAK-MCS) inherits its former multi-point enrichment algorithm allowing to add several points at each iteration step, and provide an estimated failure probability based on the Gaussian nature of the Kriging surrogate. Both the efficiency and the accuracy of the proposed method are showcased through its application to two to eight dimensional analytic examples, characterized by very low failure probabilities. Numerical experiments conducted with *unfavorable* initial *Design of Experiment* suggests the ability of the proposed method to detect failure domains [30].

5.6.4. An Efficient Kriging-Based Extreme Quantile Estimation suitable for expensive performance function

N. Razaaly, P.M. Congedo

We propose here a method for fast estimation of the quantiles associated with very small levels of probability, where the scalar performance function J is complex (e.g. output of an expensive-to-run finite element model), under a probability measure that can be recast as a multivariate standard Gaussian law using an isoprobabilistic transformation. A surrogate-based approach (Gaussian Processes) combined with adaptive experimental designs allows to iteratively increase the accuracy of the surrogate while keeping the overall number of J evaluations low. Direct use of Monte-Carlo simulation even on the surrogate model being too expensive, the key idea consists in using an Importance Sampling method based on an isotropic centered Gaussian with large Standard deviation permitting a cheap estimation of the quantiles of the surrogate. Similar to the strategy presented by Schobi and Sudret (2016), the surrogate is adaptively refined using a parallel infill refinement of an algorithm suitable for very small failure probability. We finally elaborate a multi-quantile selection approach allowing to exploit high-performance computing architectures further. We illustrate the performances of the proposed method on several two and six-dimensional cases. Accurate results are obtained with less than 100 evaluations of J. An article on this topic is under preparation.

5.7. Shape optimization under uncertainties

5.7.1. Non-Parametric Measure Approximations for Constrained Multi-Objective Optimisation under Uncertainty

M. Rivier, P.M. Congedo

In this paper, we propose non-parametric estimations of robustness and reliability measures to solve constrained multi-objective optimisation under uncertainty. These approximations with tunable fidelity permit to capture the Pareto front in a parsimonious way, and can be exploited within an adaptive refinement strategy. First, we build a non-Gaussian surrogate model of the objectives and constraints, allowing for more representativeness and detecting potential correlations. Additionally, we illustrate an efficient approach for obtaining joint representations of these robustness and reliability measures, which discriminates more sharply the Pareto-optimal designs from the others. Secondly, we propose an adaptive refinement strategy, using these tunable fidelity approximations to drive the computational effort towards the computation of the optimal area. To this extent, an adapted Pareto dominance rule and Pareto optimal probability computation are formulated. We assess the performance of the proposed strategy on several analytical test-cases against classical approaches in terms of the average distance to the Pareto front. Finally, we illustrate the performances of the method on the case of shape optimisation under uncertainty of an Organic Rankine Cycle turbine [26].

5.7.2. Optimization under Uncertainty of Large Dimensional Problems usingQuantile Bayesian Regression

C. Sabater, O. Le Maitre, P.M. Congedo, S. Goertz

When dealing with robust optimization problems, surrogate models are traditionally constructed to efficiently obtain the statistics of the random variable. However, when a large number of uncertainties are present, the required number of training samples to construct an accurate surrogate generally increases exponentially. The use of surrogates also requires the parametrization of the uncertainties. We present a novel approach for robust design insensitive to the number of uncertainties and that is able to deal with non-parametric uncertainties by leveraging a Bayesian formulation of quantile regression. The method does not require the use of any surrogate in the stochastic space. It is able to globally predict at every design point any given quantile of the random variable. In addition, it provides an estimation of the error in this prediction due to the limited sampling by making use of the posterior distribution of the model parameters.The framework includes an active infill that efficiently balances exploration with exploitation and accelerates the optimization process by increasing the accuracy of the statistic in the regions of interest. We validate the method in test functions and observe good convergence properties towards the determination of the location of the global optima. The framework is applied towards the aerodynamic robust design of an airfoil with a shock control bump under 382 geometrical and operational uncertainties. The framework is able to efficiently find the optimum configuration in complex, large-scale problems. An article on this topic is under preparation.

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

5.8.1. Multi-fidelity surrogate-based optimization of transonic and supersonic axial turbines profiles

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

This study presents a multifidelity surrogate-based approach for the optimization of the LS89 high pressure axial turbine vane to significantly reduce the computational cost associated to high fidelity CFD simulations while exploiting models of lower fidelity. A cokriging method is used to simultaneously take into account quantities of interest (QoI) coming from models of different fidelities providing a global surrogate model. A classic bayesian global optimization method permits to iteratively propose desing of interest. It relies on the maximization of the so-called Expected Improvement criterion. A geometrical parametrization technique based on B-splines is considered to describe the profile geometry. The mass-flow rate and the outlet angle are constrained. The optimization study reveals significant reduction in computational cost w.r.t. classic optimization frameworks based on a single fidelity, such as, adjoint-based and gradient-free methods, while providing similar improvements in term of fitness functions [23].

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].

Our goal is to extend Tapenade for C++. We further developed our external parser for C++, built on top of Clang-LLVM https://clang.llvm.org/. This parser is now connected to the input formalism "IL" of Tapenade. Tapenade now manages enough constructs of Object languages to be able to build its own Internal Representation (IR) and to regenerate back from the IR a non-transformed C++ source.

In the present development stage, this back-and-forth chain works on several small C++ codes. Still, many issues remain on the large example provided by the ABS team. We are working to solve those progressively. The lack of serious development documentation on the Clang internals obviously doesn't help.

The next development stage will be to adapt the analysis and differentiation components of Tapenade to the new Object constructs of the IR. This development has not started yet. Upstream this development, we need to devise an extended AD model correspondingly. This research part is in progress.

6.2. AD of mixed-language codes

Participants: Valérie Pascual, Laurent Hascoët.

We extend Tapenade to differentiate codes that mix different languages, for both tangent and adjoint modes of AD. Our motivating application is Calculix, a 3-D Structural Finite Element code that mixes Fortran and C. This year we improved the memory representation of Tapenade's IR to handle the C-Fortran memory correspondence (commons, structs...) defined by the Fortran standard.

C files (aka "translation units") and Fortran modules are two instances of the more general notion of "package" for which we have developed a unified representation in Tapenade, that also handles C++ namespaces.

6.3. Application to large industrial codes

Participants: Valérie Pascual, Laurent Hascoët, Bruno Maugars [ONERA], Sébastien Bourasseau [ONERA], Cédric Content [ONERA], Jose I. Cardesa [IMFT], Christophe Airiau [IMFT].

We support industrial users with their first experiments of Algorithmic Differentiation of large in-house codes. This concerned two industrial codes this year.

One application is with ONERA on their ElsA CFD platform (Fortran 90). This is the continuation of a collaboration started in 2018. Both tangent and adjoint models of the kernel of ElsA were built successfully with Tapenade. This year's work was mostly about improving efficiency. It is worth noticing that this application was performed inside ONERA by ONERA engineers (Bruno Maugars, Sébastien Bourasseau, Cédric Content) with no need for installation of ElsA inside Inria. We take this as a sign of maturity of Tapenade. Our contribution is driven by development meetings, in which we point out some strategies and tool options to improve efficiency of the adjoint code. As a result from these discussions, we developed improved strategies and AD model, that will be useful to other tools. These improvements deal mostly with the adjoint of vectorized code. We prepared together an aticle that describes the architecture of a modular and AD-friendly ElsA, together with the corresponding extensions of the AD model of Tapenade. This article has been submitted to "Computers and Fluids".

The other application ultimately targets AD of the “Jaguar” code, developed jointly by ONERA, CERFACS, and IMFT in Toulouse. This is a collaboration with Jose I. Cardesa and Christophe Airiau, both at IMFT. After a relatively easy tangent differentiation, most of the effort was devoted to obtaining a running and efficient adjoint code. Not too surprisingly, the main source of trouble was the Message-Passing parallel aspect on the application code. This underlined a lack of debugging support for adjoint-differentiated code. Given the run-time of the simulation that we consider (from hours to a few days on a 4110 processors platform), efficiency is crucial. We used the optimal binomial checkpointing scheme at the time-stepping level. However, performance of the adjoint code can probably be improved further with a better checkpointing scheme on the call tree. This calls in particular for AD-specific performance profiling tools, that we are planning to develop. We prepared together an article that describes this succesful experiment, which is now submitted to “Journal of Computational Science”.

Two collaborations are in preparation for next year, one with Jan Hueckelheim at Argonne National Lab. about SIMD parallel codes, and one with Stefano Carli at KU Leuven about adjoint AD of the plasma code SOLPS-ITER.

6.4. Control of approximation errors

Participants: Alain Dervieux, Loic Frazza [Gamma3 team, Inria-Saclay], Adrien Loseille [Gamma3 team, Inria-Saclay], Frédéric Alauzet [Gamma3 team, Inria-Saclay], Anca Belme [university of Paris 6], 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, we published the final revised versions of two conference papers [23], [21], we published in a journal the final version of the adjoint-based mesh adaptation for Navier-Stokes flows [16]), and we published in “Numerical Methods in Fluids” a work on nonlinear correctors extending [22]. Let us also mention the final publication 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) in which we have contributed chapters 20, 21, 45, and 48.

The monography on mesh adaptation currently being written by Alauzet, Loseille, Koobus and Dervieux now involves all its chapters (14 chapters) and is being finalized.

6.5. Turbulence models

Participants: Alain Dervieux, Bruno Koobus, Stephen Wornom.

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 models. These are mainly vortical separated regions as assumed in one of the most popular hybrid models, the hybrid Detached Eddy Simulation (DES) 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.

We have developed a new model relying on the hybridation of a DES model based on a k-ϵ closure with our dynamic VMS model [13] [11]. Our purpose is to propose a model rather predictive in condition where the engineer has not much information concerning the turbulence in the flow under study. This year, we continued to improve this model and to test it for a large set of configurations with Reynolds numbers ranging from low (laminar flows) to very large.

6.6. High order approximations

Participants: Alain Dervieux, Bruno Koobus, Stephen Wornom, Tanya Kozubskaya [Keldysh Institute of Russian Academy].

High order approximations for compressible flows on unstructured meshes are facing many constraints that increase their complexity i.e. their computational cost. This is clear for the largest class of approximation, the class of k-exact schemes, which rely on a local polynomial representation of degree k. We are investigating schemes which would solve as efficiently as possible the dilemma of choosing between an approximation with a representation inside macro-elements which finally constrains the mesh, and a representation around each individual cell, as in vertex formulations. This is a cooperation with the Keldysh Institute of Russian Academy which whom we have already developed several families of superconvergent schemes.

6.7. Aeroacoustics

Participants: Alain Dervieux, Bruno Koobus, Stephen Wornom, Tanya Kozubskaya [Keldysh Institute of Russian Academy].

The progress in highly accurate schemes for compressible flows on unstructured meshes (together with advances in massive parallelization of these schemes) allows us to solve problems previously out of reach. The three teams of Montpellier university (coordinator), Inria-Sophia and Keldysh Institute of Moscow have written a proposal for cooperation on the subject of the extension of these methods to simulate the noise emission of rotating machines (helicopters, future aerial vehicles, unmanned aerial vehicles, wind turbines...). The proposal has been selected by ANR and RSF (Russian Science Foundation) for support for a program duration of 4 years.

ELAN Project-Team

7. New Results

7.1. Static simulation of thin elastic ribbons

Participants: Raphaël Charrondière, Florence Bertails-Descoubes, Victor Romero.

In collaboration with Sébastien Neukirch (Sorbonne Université, Institut Jean le Rond d'Alembert), we have proposed a robust and efficient numerical model to compute stable equilibrium configurations of thin elastic ribbons featuring arbitrarily curved natural shapes. Our spatial discretization scheme relies on elements characterized by a linear normal curvature and a quadratic geodesic torsion with respect to arc length. Such a high-order discretization allows for a great diversity of kinematic representations, while guaranteeing the ribbon to remain perfectly inextensible. Stable equilibria are calculated by minimizing gravitational and elastic energies of the ribbon, under a developability constraint. This work is currently under review in a journal of Mechanics. Some preliminary results have already been communicated about in two French congresses, one in Mechanics [6] and one in Computer Graphics [7] (best paper award).

7.2. Video-based measurement of the friction coefficient between cloth and a substrate

Participants: Haroon Rasheed, Victor Romero, Florence Bertails-Descoubes.

In collaboration with Arnaud Lazarus (Sorbonne Université, Institut Jean le Rond d'Alembert), Jean-Sébastien Franco and Stefanie Wuhrer (Inria, Morphéo team), we have investigated a first non-invasive measurement network for estimating cloth friction at contact with a substrate. Our network was trained on data exclusively generated by the solver ARGUS co-developed by the ELAN team, which we have carefully validated against real experiments under controlled conditions. We have shown promising friction measurement results on multiple real cloth samples contacting various kinds of substrates, by comparing our estimations based on a simple video acquisition protocol against standard measurements. This work has been submitted in late 2019 for publication in a Computer Vision conference, and some preliminary results have been communicated about in a mechanical congress [4].

7.3. Willmore flow simulation with diffusion-redistanciation numerical schemes

Participant: Thibaut Metivet.

In collaboration with Arnaud Sengers (Université Claude Bernard), Emmanuel Maitre (Laboratoire Jean Kuntzmann, Grenoble INP) and Mourad Ismail (Laboratoire Interdisciplinaire de Physique, UGA), we have proposed original diffusion-redistanciation numerical schemes to compute the static shapes of elastic membranes with bending stiffness under constant area constraints. This numerical method relies on an implicit representation of the surface which is used as an initial condition for diffusion-like equations. This allows to circumvent the usual difficulties pertaining to the high geometrical order and non-linearities of the bending energy and to benefit from the robustness of discretised diffusion operators. We have implemented the schemes within the finite element library Feel++ and studied the numerical convergence properties in 2D and 3D. We have also validated our method using comparative benchmarks computed with standard approaches. This work has led to the PhD defense of Arnaud Sengers [35] and a publication is under preparation.

GAMMA Project-Team

4. New Results

4.1. The meshing bible

Participants: Paul Louis George [correspondant], Frédéric Alauzet, Adrien Loseille, Loïc Maréchal.

Un projet important, initié en 2017, et toujours actif en 2020, 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.

4.2. Pixel-exact rendering for high-order meshes and solutions

Participants: Adrien Loseille [correspondant], Rémi Feuillet, Matthieu Maunoury.

Classic visualization software like ParaView [64], TecPlot [88], FieldView [60], Ensight [42], Medit [50], Vizir (OpenGL legacy based version) [67], Gmsh [57], ...historically rely on the display of linear triangles with linear solutions on it. More precisely, each element of the mesh is divided into a set of elementary triangles. At each vertex of the elementary triangle is attached a value and an associated color. The value and the color inside the triangle is then deduced by a linear interpolation inside the triangle. With the increase of high-order methods and high-order meshes, these softwares adapted their technology by using subdivision methods. If a mesh has high-order elements, these elements are subdivided into a set of linear triangles in order to approximate the shape of the high-order element [93]. Likewise, if a mesh has a high-order solution on it, each element is subdivided into smaller linear triangles in order to approximate the rendering of the high-order solution on it. The subdivision process can be really expensive if it is done in a naive way. For

this reason, mesh adaptation procedures [80], [70], [71] are used to efficiently render high-order solutions and high-order elements using the standard linear rendering approaches. Even when optimized these approaches do have a huge RAM memory footprint as the subdivision is done on CPU in a preprocessing step. Also the adaptive subdivision process can be dependent on the palette (*i.e.* the range of values where the solution is studied) as the color only vary when the associated value is in this range. In this case, a change of palette inevitably imposes a new adaptation process. Finally, the use of a non conforming mesh adaptation can lead to a discontinuous rendering for a continuous solution.
Other approaches are specifically devoted to high-order solutions and are based on ray casting [75], [76], [78]. The idea is for a given pixel, to find exactly its color. To do so, for each pixel, rays are cast from the position of the screen in the physical space and their intersection with the scene determines the color for the pixel. If high-order features are taken into account, it determines the color exactly for this pixel. However, this method is based on two non-linear problems: the root-finding problem and the inversion of the geometrical mapping. These problems are really costly and do not compete with the interactivity of the standard linear rendering methods even when these are called with a subdivision process unless they are done conjointly on the GPU. However, synchronization between GPU and `OpenGL` buffer are non-trivial combination.
The proposed method intends to be a good compromise between both methods. It does guarantee pixel-exact rendering on linear elements without extra subdivision or ray casting and it keeps the interactivity of a classical method. Moreover, the subdivision of the curved entities is done on the fly on GPU which leaves the RAM memory footprint at the size of the loaded mesh.

4.3. High-order mesh generation

Participants: Frédéric Alauzet [correspondant], Adrien Loseille, Rémi Feuillet, Dave Marcum, Lucien Rochery.

For years, the resolution of numerical methods has consisted in solving Partial Derivative Equations by means of a piecewise linear representation of the physical phenomenon on linear meshes. This choice was merely driven by computational limitations. With the increase of the computational capabilities, it became possible to increase the polynomial order of the solution while keeping the mesh linear. This was motivated by the fact that even if the increase of the polynomial order requires more computational resources per iteration of the solver, it yields a faster convergence of the approximation error [0] [92] and it enables to keep track of unsteady features for a longer time and with a coarser mesh than with a linear approximation of the solution. However, in [46], [65], it was theoretically shown that for elliptic problems the optimal convergence rate for a high-order method was obtained with a curved boundary of the same order and in [44], evidence was given that without a high-order representation of the boundary the studied physical phenomenon was not exactly solved using a high-order method. In [95], it was even highlighted that, in some cases, the order of the mesh should be of a higher degree than the one of the solver. In other words, if the used mesh is not a high-order mesh, then the obtained high-order solution will never reliably represent the physical phenomenon.

Based on these issues, the development of high-order mesh generation procedures appears mandatory. To generate high-order meshes, several approaches exist. The first approach was tackled twenty years ago [47] for both surface and volume meshing. At this moment the idea was to use all the meshing tools to get a valid high-order mesh. The same problem was revisited a few years later in [86] for bio-medical applications. In these first approaches and in all the following, the underlying idea is to use a linear mesh and elevate it to the desired order. Some make use of a PDE or variational approach to do so [39], [79], [48], [73], [91], [94], [58], others are based on optimization and smoothing operations and start from a linear mesh with a constrained high-order curved boundary in order to generate a suitable high-order mesh [62], [51], [89]. Also, when dealing with Navier-Stokes equations, the question of generating curved boundary layer meshes (also called viscous meshes) appears. Most of the time, dedicated approaches are set-up to deal with this problem [74], [63]. In all these techniques, the key feature is to find the best deformation to be applied to the linear mesh and to optimize it. The prerequisite of these methods is that the initial boundary is curved and will be used as an input data. A natural question is consequently to study an optimal position of the high-order nodes on the curved boundary

[0] The order of convergence is the degree of the polynomial approximation plus one.

starting from an initial linear or high-order boundary mesh. This can be done in a coupled way with the volume [81], [90] or in a preprocessing phase [82], [83]. In this process, the position of the nodes is set by projection onto the CAD geometry or by minimization of an error between the surface mesh and the CAD surface. Note that the vertices of the boundary mesh can move as well during the process. In the case of an initial linear boundary mesh with absence of a CAD geometry, some approaches based on normal reconstructions can be used to create a surrogate for the CAD model [93], [59]. Finally, a last question remains when dealing with such high-order meshes: Given a set of degrees of freedom, is the definition of these objects always valid ?. Until the work presented in [55], [61], [52], no real approach was proposed to deal in a robust way with the validity of high-order elements. The novelty of these approaches was to see the geometrical elements and their Jacobian as Bézier entities. Based on the properties of the Bézier representation, the validity of the element is concluded in a robust sense, while the other methods were only using a sampling of the Jacobian to conclude about its sign without any warranty on the whole validity of the elements.
In this context, several issues have been addressed : the analogy between high-order and Bézier elements, the development of high-order error estimates suitable for parametric high-order surface mesh generation andthe generalization of mesh optimization operators and their applications to curved mesh generation, moving-mesh methods, boundary layer mesh generation and mesh adaptation.

4.4. Unstructured anisotropic mesh adaptation for 3D RANS turbomachinery applications

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

The scope of this paper is to demonstrate the viability and efficiency of unstructured anisotropic mesh adaptation techniques to turbomachinery applications. The main difficulty in turbomachinery is the periodicity of the domain that must be taken into account inthe solution mesh-adaptive process. The periodicity is strongly enforced in the flow solver using ghost cells to minimize the impact on the source code. For the mesh adaptation, the local remeshing is done in two steps. First, the inner domain is remeshed with frozen periodic frontiers, and, second, the periodic surfaces are remeshed after moving geometrice ntities from one side of the domain to the other. One of the main goal of this work is to demonstrate how mesh adaptation, thanks to its automation, is able to generate meshes that are extremely difficult to envision and almost impossible to generate manually. This study only considers feature-based error estimate based on the standard multi-scale Lpinterpolation error estimate. We presents all the specific modifications that have been introduced in the adaptive process to deal with periodic simulations used for turbomachinery applications. The periodic mesh adaptation strategy is then tested and validated on the LS89 high pressure axial turbine vane and the NASA Rotor 37 test cases.

4.5. Hybrid mesh adaptation for CFD simulations

Participants: Frédéric Alauzet [correspondant], Lucille Tenkès, Julien Vanharen.

The aim of mesh adaptation is to generate the optimal mesh to perform a specific numerical simulation. It is nowadays a mature tool which is mathematically well-posed and fully automatic regarding tetrahedral meshes. Yet, there is still a strong demand for structured meshes, as many numerical schemes have proven to be more accurate on quadrilateral meshes than on triangular meshes, and as many favor structured elements in the boundary layer instead of tetrahedra to simulate viscous turbulent flows. Since no method can automatically provide pure hexahedral adapted meshes respecting alignment constraints, one solution is to use hybrid meshes, *i.e.* meshes containing both structured and unstructured elements. Accordingly, the following work focuses on hybrid metric-based mesh adaptation and CFD simulation on such meshes. Regarding hybrid mesh generation, the method relies on a preliminary mesh obtained through so-called metric-aligned and metric-orthogonal approaches. These approaches utilize the directional information held by a prescribed metric-field to generate right angled elements, that can be combined into structured elements to form a hybrid mesh. The result highly depends on the quality of the metric field. Thus, emphasis is put on the size gradation control performed beforehand. This process is re-designed to favor metric-orthogonal meshes. To validate the method, some CFD simulations are performed. The modifications brought to the existing Finite Volume solver to enable such computations has been developed.

4.6. Anisotropic mesh adaptation for fluid-structure interactions

Participants: Frédéric Alauzet, Adrien Loseille, Julien Vanharen [correspondant].

A new strategy 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 P^1 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.

MATHERIALS Project-Team

6. New Results

6.1. Electronic structure calculations and related problems

Participants: Robert Benda, Éric Cancès, Virginie Ehrlacher, Luca Gorini, Gaspard Kemlin, Claude Le Bris, Antoine Levitt, Sami Siraj-Dine, Gabriel Stoltz.

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 (rHF) approximation, a model striking a good balance between mathematical tractability and the ability to reproduce qualitatively complex effects.

In collaboration with L. Cao, E. Cancès and G. Stoltz have studied the nuclear dynamics of infinite crystals with local defects within the Born-Oppenheimer approximation, using the reduced Hartree-Fock model to compute the electronic ground state. In this model, nuclei obey an autonomous classical Hamiltonian dynamics on a potential energy surface obtained by rHF electronic ground-state calculations. One of the main motivations for this work is to study the *nonlinear* collective excitations of nuclei in a crystal, in order to go beyond the simple harmonic approximation of non-interacting phonons. rHF ground states associated with generic nuclear displacements with respect to the periodic configuration are not mathematically well-defined at the time of writing. However, by relying on results by Cancès, Deleurence and Lewin for the rHF ground states of crystals with local defects, it is possible to study the fully nonlinear rHF Born-Oppenheimer dynamics of nuclei in the neighborhood of an equilibrium periodic configuration of a crystal. A Hilbert space of admissible nuclear displacements, and an infinite-dimensional Hamiltonian describing the dynamics of nuclei can then be defined. For small initial data, it is proved that the Cauchy problem associated with this Hamiltonian dynamics is well posed for short times (see the PhD thesis of Lingling Cao). The existence and uniqueness for arbitrary initial data, and/or long times requires a perturbation analysis of the rHF model when the Fermi level is occupied, which is work in progress.

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 (Besançon), B. Stamm (Aachen, Germany), and M. Vohralìk (Inria SERENA), they have designed *a posteriori* error estimates for conforming numerical approximation of eigenvalue clusters of second-order self-adjoint operators on bounded domains [44]. Given a cluster of eigenvalues, they have estimated the error in the sum of the eigenvalues, as well as the error in the eigenvectors represented through the density matrix, i.e. the orthogonal projector on the associated eigenspace. This allows them to deal with degenerate (multiple) eigenvalues within this framework. The bounds are guaranteed and converge at the same rate as the exact error. They can be turned into fully computable bounds as soon as an estimate on the dual norm of the residual is available, which is notably the case (i) for the Laplace eigenvalue problem discretized with conforming finite elements, and (ii) for a Schrödinger operator with periodic boundary conditions discretized with plane waves.

R. Benda, E. Cancès and B. Lebental (Ecole Polytechnique) have initiated the design and analysis of multiscale models for the electrical conductivity of networks of functionalized carbon nanotubes. Such devices are used as nanosensors, for instance to monitor the quality of water. In [11], they study by means of Monte-Carlo numerical simulations the resistance of two-dimensional random percolating networks of stick, widthless nanowires. They use the multi-nodal representation (MNR) to model a nanowire network as a graph. They derive numerically from this model the expression of the total resistance as a function of all meaningful parameters, geometrical and physical, over a wide range of variation for each. They justify their choice of non-dimensional variables applying Buckingham π-theorem. The effective resistance of 2D random percolating networks of nanowires is found to have a nice expression in terms of the geometrical parameters (number of wires, aspect ratio of electrode separation over wire length) and the physical parameters (nanowire linear resistance per unit length, nanowire/nanowire contact resistance, metallic electrode/nanowire contact resistance). The dependence of the resistance on the geometry of the network, on the one hand, and on the physical parameters (values of the resistances), on the other hand, is thus clearly separated thanks to this expression, much simpler than the previously reported analytical expressions. In parallel, atomic scale models based on electronic structure theory are being developed to parameterize these mesoscale models (PhD thesis of R. Benda).

C. Le Bris has pursued his long term collaboration with Pierre Rouchon (Ecole des Mines de Paris and Inria QUANTIC) on the study of high dimensional Lindblad type equations at play in the modelling of open quantum systems. They have co-supervised the M2 internship of Luca Gorini, that was focused on the simulation of some simple quantum gates, and has investigated several discretization strategies based upon the choice of suitable basis sets.

V. Ehrlacher, L. Grigori (Inria ALPINES), D. Lombardi (Inria COMMEDIA) and H. Song (Inria ALPINES) have designed a new numerical method for the compression of high-order tensors [49]. The principle of the algorithm consists in constructing an optimal partition of the set of indices of the tensor, and construct an approximation of the tensor on each indices subdomain by means of an adapted High-Order Singular Value Decomposition. This method was used, among other examples, for the reduction of the solution of the Vlasov-Poisson system, and enabled to reach very significant compression factors. They also obtained very encouraging results on the compression of the Coulomb potential, which could be very interesting with a view to the resolution of the time-dependent Schrödinger equation in high dimension, which is currently work in progress.

A. Alfonsi, R. Coyaud (Ecole des Ponts), V. Ehrlacher and D. Lombardi (Inria COMMEDIA) studied a different approach for discretizing optimal transport problems, which relies in relaxing the marginal constraints in a finite number of marginal moment constraints, while keeping an infinite state space [40]. The advantage of such an approach is that the approximate solution of the multi-marginal optimal transport problem with Coulomb cost, which is the semi-classical limit of the so-called Lévy-Lieb functional, can be represented as a discrete measure charging a low number of points, thus avoiding the curse of dimensionality when the number of electrons is large.

M. Herbst and his collaborators have developed the `adcc` Python/C++ software package for performing excited state calculations based on algebraic-diagrammatic construction methods. It connects to four SCF packages (pyscf, psifour, molsturm and veloxchem), allows the inclusion of environmental effects through implicit or explicit solvent models, and implements methods up to third order in perturbation theory. Its features are summarized in [54].

6.2. Computational Statistical Physics

Participants: Manon Baudel, Qiming Du, Grégoire Ferré, Frédéric Legoll, Tony Lelièvre, Mouad Ramil, Geneviève Robin, Laura Silva Lopes, Gabriel Stoltz.

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 efficient computation of dynamical properties which requires to sample metastable trajectories; (iii) the simulation of nonequilibrium systems and the computation of transport coefficients; (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

The work [52] by G. Ferré and G. Stoltz considers fluctuations of empirical averages for stochastic differential equations. Such averages are commonly used to compute ergodic averages in statistical physics in order to estimate macroscopic quantities, but they are subject to fluctuations. If small deviations are described by the central limit theorem, important fluctuations enter the large deviations framework. This theory is well understood when considering bounded observables of a stochastic differential equation, but quantities of interest are generally unbounded. The authors identify the class of unbounded functions which enter the "usual" regime of large deviations. The answer is not trivial, and suggests that many physical observables satisfy another type of large deviations, which leads to further works. Additionally, the influence of irreversibility on the fluctuations was studied by providing a mathematical illustration of the second law of thermodynamics, stating that irreversible dynamics generate more entropy, or more disorder, than reversible ones.

The team also pursued its endeavour to study and improve free energy biasing techniques, such as adaptive biasing force or metadynamics. The gist of these techniques is to bias the original metastable dynamics used to sample the target probability measure in the configuration space by an approximation of the free energy along well-chosen reaction coordinates. This approximation is built on the fly, using empirical measures over replicas, or occupations measures over the trajectories of the replicas. Two works have been performed on such methods

- First, in [50], V. Ehrlacher, T. Lelièvre and P. Monmarché (Sorbonne Université) have developed a new numerical method in order to compute the free energy and the biased potential given by the Adaptive Biasing Force method in the case where the number of reaction cordinates in the system is too large to apply standard grid-based approximation techniques. The algorithm uses a greedy algorithm and a tensor product approximation. Convergence proofs of both the underlying ABF technique (which uses an unbiased occupation measure) and the greedy tensor-product approximation are provided.
- Second, in [55], T. Lelièvre together with B. Jourdain (Ecole des Ponts) and P.-A. Zitt (Université Paris Est) have used a parallel between metadynamics and self interacting models for polymers to study the longtime convergence of the original metadynamics algorithm in the adiabatic setting, namely when the dynamics along the collective variables decouple from the dynamics along the other degrees of freedom. The bias which is introduced when the adiabatic assumption does not hold is also discussed.

The team has also considered new applications in terms of sampling, and the analysis of related sampling methods:

- For large scale Bayesian inference, B. Leimkuhler (Edinburgh, United Kingdom), M. Sachs (Duke, USA) and G. Stoltz have studied in [57] the convergence of Adaptive Langevin dynamics, which is a method for sampling the Boltzmann-Gibbs distribution at a prescribed temperature in cases where the potential gradient is subject to stochastic perturbation of unknown magnitude. The method replaces the friction in underdamped Langevin dynamics with a dynamical variable, updated according to a negative feedback loop control law as in the Nose-Hoover thermostat. Hypocoercive techniques allow to show that the law of Adaptive Langevin dynamics converges exponentially rapidly to the stationary distribution, with a rate that can be quantified in terms of the key parameters of the dynamics. This implies in particular that a central limit theorem holds for the time averages computed along a stochastic path.
- For the simulation of log-gases, G. Ferré and G. Stoltz have studied in [46] with D. Chafaï (Université Paris Dauphine) a follow up to a former project on the efficient simulation of Coulomb and logarithmic gases. A previous work has demonstrated the usefulness of Hybrid Monte Carlo techniques for sampling the invariant measure of such gases. Gases under constraint are now considered. First, the algorithm proposed in [31] was used to numerically explore the situation. Then, large deviations techniques were employed to study the limiting behaviour of the conditioned gas when the number of particles gets large. For a class of constraints, the equation solved by the limiting empirical density shows in particular cases a spectacular behaviour. This work suggests to further explore some research paths, such as the limiting distribution for large constraints.

6.2.2. Sampling of dynamical properties and rare events

In the preprint [48], T. Lelièvre uses the quasi-stationary distribution approach to study the first exit point distribution from a bounded domain of the overdamped Langevin dynamics, in collaboration with G. Di Gesù (TU Wien, Austria), B. Nectoux (Université Blaise Pascal) and D. Le Peutrec (Université Paris-Sud). The quasi-stationary distribution approach has been developed by T. Lelièvre and collaborators over the past years in order to rigorously model the exit event from a metastable state by a jump Markov process, and to study this exit event in the small temperature regime. In [48], the authors prove that in the small temperature regime and under rather general assumptions on the initial conditions and on the potential function, the support of the distribution of the first exit point concentrates on some points realizing the minimum of the potential on the boundary. The proof relies on tools to study tunnelling effects in semi-classical analysis. This preprint has been divided into two separate articles for publication: the first one [22] has been accepted for publication; the second one is currently under review.

6.2.3. Nonequilibrium systems and computation of transport coefficients

Stemming from the IHP trimester "Stochastic Dynamics Out of Equilibrium" held at Institut Henri Poincare in April-July 2017, a collection of contributions has been grouped in a volume of proceedings [38], focusing on aspects of nonequilibrium dynamics and its ongoing developments. This volume has been edited by G. Giacomin (Universite Paris Diderot), S. Olla (Université Paris Dauphine), E. Saada (CNRS and Université Paris Descartes), H. Sophn (TU Munich, Germany) and G. Stoltz. It includes contributions from various events relating to three domains: (i) transport in non-equilibrium statistical mechanics; (ii) the design of more efficient simulation methods; (iii) life sciences.

In addition, P. Plechac (University of Delaware, USA), T. Wang (Army Research Lab, USA) and G. Stoltz have considered in [61] numerical schemes for computing the linear response of steady-state averages of stochastic dynamics with respect to a perturbation of the drift part of the stochastic differential equation. The schemes are based on Girsanov's change-of-measure theory to reweight trajectories with factors derived from a linearization of the Girsanov weights. Both the discretization error and the finite time approximation error have been investigated. The designed numerical schemes have been shown to be of bounded variance with respect to the integration time, which is a desirable feature for long time simulation. The discretization error has been shown to be improved to second order accuracy in the time step by modifying the weight process in an appropriate way.

6.2.4. Coarse-graining

Two works have been done to explore new methods to define "good" reaction coordinates:

- The estimation of the Poincaré constant of a given probability measure allows to quantify the typical convergence rate of reversible diffusions to their equilibrium measure. Loucas Pillaud-Vivien, F. Bach and A. Rudi (Inria SIERRA), together with T. Lelièvre and G. Stoltz, have shown in [58], both theoretically and experimentally how to estimate the Poincaré constant given sufficiently many samples of the probability measure under consideration, using reproducing Hilbert kernel spaces. As a by-product of this estimation, they have also derived an algorithm that captures a low dimensional representation of the data by finding directions which are difficult to sample – reaction coordinates in the language of molecular dynamics. This amounts to finding the marginal of the high dimensional sampled measure for which the Poincaré constant is the largest possible.
- In [60], T. Lelièvre together with B. Leimkuhler and Z. Trstanova (University of Edinburgh, Scotland) has explored numerically the interest of using diffusion maps to define reaction coordinates or metastable states. Diffusion maps approximate the generator of Langevin dynamics from simulation data, and the idea is thus to use the eigenvalues and eigenvectors to build coarse-grained variables. They have also discussed the use of diffusion maps to define local reaction coordinates within the metastable sets, formalising the locality via the concept of quasi-stationary distribution and justifying the convergence of diffusion maps applied to samples within a metastable set.

Another coarse-graining procedure was considered to justify the approximation of an infinite system of ordinary differential equations (the Becker-Doring equations, describing coagulation/fragmentation processes of species of integer sizes) in terms of a partial differential equation. Formal Taylor expansions motivate that the dynamics at large sizes should be dictated by an advection-diffusion equation, called Fokker-Planck equation. P. Terrier and G. Stoltz rigorously proved in [59] the link between these two descriptions for evolutions on finite times rather than in some hydrodynamic limit, motivated by the results of numerical simulations and the construction of dedicated algorithms based on splitting strategies. In fact, the Becker-Doring equations and the Fokker-Planck equation are related through some pure diffusion with unbounded diffusion coefficient. The crucial point in the analysis is to obtain decay estimates for the solution of this pure diffusion and its derivates to control remainders in the Taylor expansions. The small parameter in this analysis is the inverse of the minimal size of the species.

6.3. Homogenization

Participants: Xavier Blanc, Virginie Ehrlacher, Olga Gorynina, Rémi Goudey, Claude Le Bris, Frédéric Legoll, Adrien Lesage, Pierre-Loïk Rothé.

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 several different directions.

6.3.1. Deterministic non-periodic systems

For linear elliptic equations with highly oscillating coefficients, X. Blanc and C. Le Bris have recently developed, in collaboration with P.-L. Lions (Collège de France), a theory in the case of periodic problems with local defects. In particular, the existence of a corrector function for such problems has been shown. More details on the quality of approximation achieved by their theory have been recently provided. The fact that a corrector exists with suitable properties indeed allows one to quantify the rate of convergence of the two-scale expansion (which uses that corrector) to the actual exact solution, as the small homogenization parameter ε vanishes. In that spirit, some of these works by X. Blanc and C. Le Bris, in collaboration with M. Josien (former PhD student in the team, now at MPI Leipzig, Germany), have been presented in [12], [13].

Also in the context of homogenization theory, O. Gorynina, C. Le Bris and F. Legoll have explored the question of how to determine the homogenized coefficient of heterogeneous media without explicitly performing an homogenization approach. This work is a follow-up on earlier works by C. Le Bris and F. Legoll in collaboration with K. Li and next S. Lemaire over the years. During the year, O. Gorynina, C. Le Bris and F. Legoll have mathematically studied a computational approach initially introduced by R. Cottereau (CNRS Marseille). This approach combines, in the Arlequin framework, the original fine-scale description of the medium (modelled by an oscillatory coefficient) with an effective description (modelled by a constant coefficient) and optimizes upon the coefficient of the effective medium to best fit the response of a purely homogeneous medium. In the limit of asymptotically infinitely fine structures, the approach yields the value of the homogenized coefficient. The aim is to mathematically study the problem and to investigate how to improve on the practical algorithm, in order to obtain a procedure as efficient as possible. Results will be presented in a couple of manuscripts in preparation.

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, and the team has proposed, over the past years, many approaches to improve on the computation of the homogenized tensor.

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 has been 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 (based on using the standard truncated corrector problem) has been designed to approximate Q and its convergence has been proven, again in a weakly stochastic setting. All these theoretical results critically depend on detailed properties of the Green function associated to the periodic operator. Second, numerical experiments in more general settings (i.e. full stochastic case) following the same approach have been performed, in order to investigate the generality of the obtained results. First, the convergence of the approximation of Q has been monitored. Second, it has been checked that the localized fluctuations of u_ε indeed become Gaussian when ε decreases, and that their variance can be related to Q. These promising numerical results, which are consistent with the theoretical results obtained in the weakly stochastic setting, are presented in a manuscript in preparation.

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 MsFEM approach uses a Galerkin approximation 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 completed the study of 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. In addition, residue type a posteriori error estimators have been proposed and certified, leading to a numerical strategy where the degree of enrichment is *locally* adapted in order to reach, at the smallest computational cost, a given error. The promising numerical results are currently being collected in a manuscript in preparation.

Many numerical analysis studies of the MsFEM are focused on obtaining a priori error bounds. In collaboration with L. Chamoin, who was on leave in the project-team a few years ago from ENS Cachan, members of the project-team have been working on a posteriori error analysis for MsFEM approaches, with the aim of developing error estimation and adaptation tools. They have extended to the MsFEM case an approach that is classical in the computational mechanics community for single scale problems, and which is based on the so-called Constitutive Relation Error (CRE). Once a numerical solution u_h has been obtained, the approach needs additional computations in order to determine a divergence-free field as close as possible to the exact flux $k\nabla u$. In the context of the MsFEM, it is important to be able to perform all expensive computations in an offline stage, independently of the right-hand side. The standard CRE approach has thus been adapted to that context. In the recent work [47], the approach has also been adapted towards the design of adaptive algorithms for specific quantities of interest (in the so-called “goal-oriented” setting). It provides an accurate estimation of the error, and leads to a discretization which is efficiently tailored to the specific quantity under consideration.

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 (see [37]). The first steps of the work of V. Ehrlacher, F. Legoll and A. Lesage, in collaboration with A. Lebée (Ecole des Ponts) have consisted in studying the homogenized limit (and the two-scale expansion) of problems posed on thin heterogeneous plates. After having considered the case of a diffusion equation, the more challenging case of elasticity has been studied. In the so-called membrane case (that is, when the loading is in the in-plane directions), an approximation result for the two-scale expansion has been obtained. Several MsFEM variants have been proposed and compared numerically. The results will be presented in a forthcoming manuscript.

6.4. Various topics

Participants: Sébastien Boyaval, Virginie Ehrlacher.

A new mathematical framework has been identified for the modelling of complex fluids in [42]. It allows one to incorporate rheological features of a real (non-ideal, visous and compressible) fluid and, at the same time, to compute flows as solution to a *hyperbolic system of conservation laws* complemented by an initial value. In [42], the framework is specified for 2D hydrostatic flows of *Maxwell fluids*, with a numerical finite-volume scheme preserving the positivity of mass and a Clausius-Duem inequality. Formally, the (macroscopic) model has a (microscopic) molecular justification using a generalized Langevin equation for the distortion of the fluid texture.

On the other hand, recall that stochastic models are also used for the numerical simulation of hydrodynamical turbulence. In particular, a generalized Langevin equation can be used to model the "thermostated" velocity fluctuations in a "stationary" turbulent flow modelled as an invariant measure. But the interest for the effective numerical simulation of turbulent flows is not fully understood yet. In [43], S. Boyaval with S. Martel and J. Reygner (Ecole des Ponts) have studied the convergence of a discretization of a 1D stochastic scalar viscous conservation laws (a toy-model), for the numerical simulation of its invariant measure.

A. Benaceur (EDF), V. Ehrlacher and A. Ern (École des Ponts and Inria SERENA) developped a new EIM/reduced-basis method [10] for the reduction of parametrized variational inequalities with nonlinear constraints, and applied this method to the reduction of contact mechanics problems with non-coincident meshes.

V. Ehrlacher, D. Lombardi (Inria COMMEDIA), O. Mula (Université Paris-Dauphine) and F-X. Vialard (Université Paris-Est) developped new model-order reduction techniques based on the use of Wasserstein spaces for transport-dominated problems [51], which gives very encouraging results on several classes of conservative transport problems like the Burger's equation. Theoretical convergence rates are proved on some particular test cases.

J. Berendsen (Chemnitz, Germany), Martin Burger (Erlangen, Germany), V. Ehrlacher, J-F. Pietschmann (Chemnitz, Germany) proved the existence and uniqueness of strong solutions and weak-strong stability in a particular system of cross-diffusion equations [41]. It is in general very difficult to obtain such kind of results for general cross-diffusion systems. The proof for the particular system studied here relies on the fact that, when all the cross-diffusion coefficients of the system are equal to the same constant, the system boils down to a set of independent heat equations, for which uniqueness of strong solutions is trivial. The uniqueness of strong solutions was proved under the assumption that the cross-diffusion coefficients should not be close enough to one another.

MEMPHIS Project-Team

7. New Results

7.1. DGDD Method for Reduced-Order Modeling of Conservation Laws

Reduced-order models are attractive method to decrease significantly the computational cost of the simulations. However, the ability of reduced-order models to accurately approximate solutions containing strong convection, sharp gradients or discontinuities can be challenging. The discontinuous Galerkin domain decomposition (DGDD) reduced model for systems of conservation laws couples at the discrete level sub-domains of high-fidelity polynomial approximation to regions of low-dimensional resolution as shown in figure 8 .

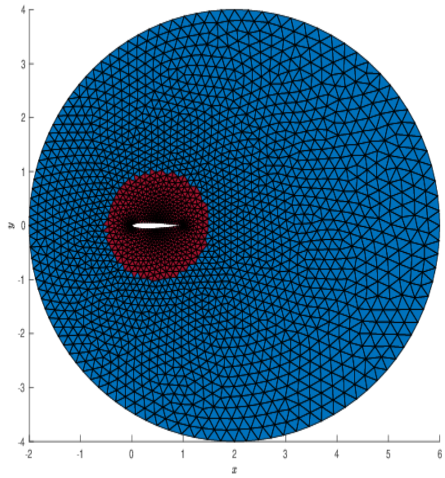


Figure 8. Decomposition of the domain: high-dimensional model (red), reduced-order model (blue).

In this approach, the high-dimensional model solves the equations where a given degree of accuracy is required, while the reduced-order model approximates the solution elsewhere. Since the high-dimensional model is used in a small part of the domain, the computational cost is significantly reduced. To perform the coupling, we develop a reduced-order model based on Proper Orthogonal Decomposition in the offline stage and on discontinuous Galerkin method in the online stage instead of the standard Galerkin method. In this way, the domain decomposition is applied transparently thought the numerical fluxes. We investigate the prediction of unsteady flows over a NACA 0012 airfoil. The results demonstrate the accuracy of the proposed method and the significant reduction of the computational cost. In the figures (9 and 10) we show examples of predictions obtained by the low-order model compared to the actual solutions as a function of the Mach number at infintiy and the angle of attack. In the last figure we present the overall space-time L^2 errors as a function of the low-dimensional space size.

7.2. Segmentation of aortic aneurism: collaboration with Nurea

Starting from February 2019, AMIES granted a one-year contract engineer in close collaboration with the Nurea start-up.

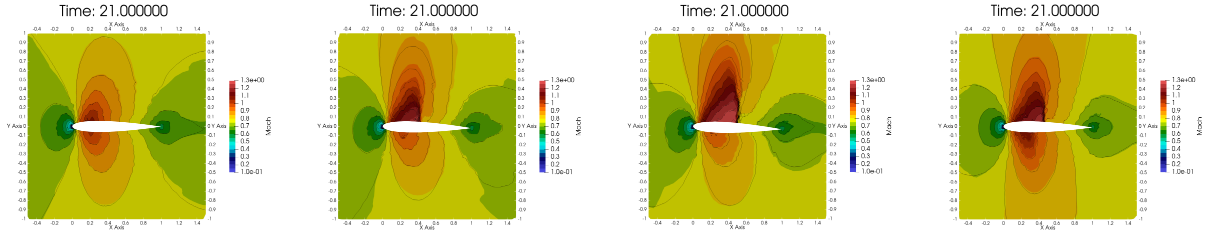


Figure 9. From left to right: $M_\infty = 0.754$ *and* $\alpha = 0.2$*,* $M_\infty = 0.763$ *and* $\alpha = 1.1$*,* $M_\infty = 0.776$ *and* $\alpha = 1.8$*,* $M_\infty = 0.784$ *and* $\alpha = 0.6$

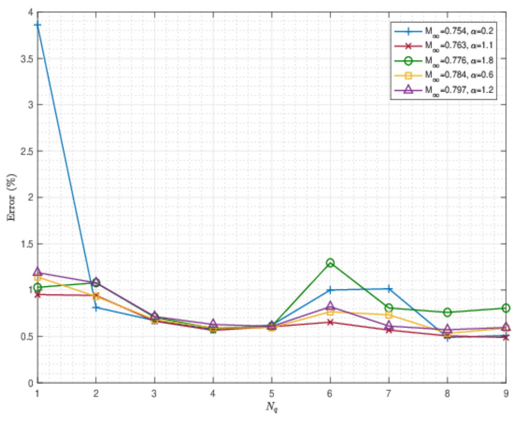


Figure 10. With $N_q = 9$ *basis functions,* ***the approximation error is less than 1% and the run time is reduced by approximately 72%*** *with respect to the high-fidelity solutions.*

The main objective of the project is to improve the quality and the robustness of automatic segmentation of aortic aneurism. An important part of the work was to decide if patient data needed to be pre-processed or not. To do so a criteron was developed to apply or not a smoothing filter. Several filters were tested and their performance were compared in order to choose the filter the more appropriate to our problem.
Another issue was the bones wrongly taken into the segmentation. A cleaning function was created to deal with it and remove the bones from the segmentation. An usual issue when working with medical images is to deal with the gradient of intensity. Existing tools need to be adapted to take into account these variations within images. This is currently worked out.
The code is implemented in C++ and mostly relies on itk and vtk libraries. An example in figure 11 .

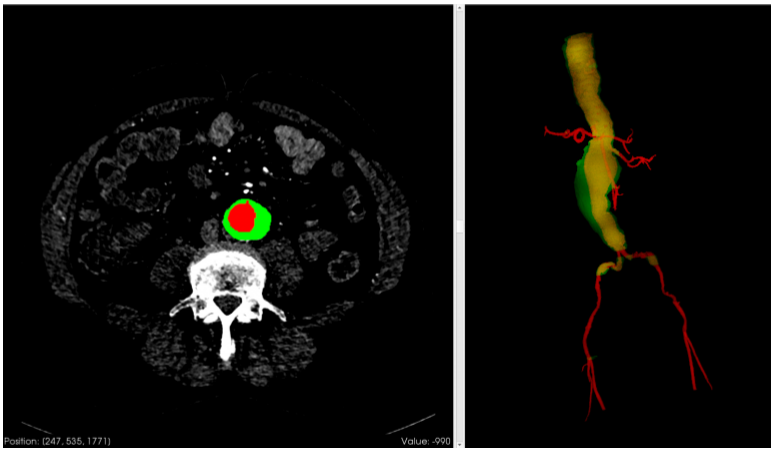


Figure 11. Example of aortic aneurism segmentation. Left: CT scan image; Right: 3D visualization. Red: blood; green: aortic wall

7.3. Fluid-structure interactions on AMR enabled quadree grids

We develop a versatile fully Eulerian method for the simulation of fluid-structure interactions. In the context of a monolithic approach, the whole system is modeled through a single continuum model. The equations are numerically solved using a finite-volume scheme with a compact stencil on AMR enabled quadtree grids where the dynamic refinement is adapted in time to the fluid-structure system.

The geometry is followed using a level-set formulation. In the Eulerian representation, a smooth Heaviside function is defined according to a level-set function on the cartesian mesh to distinguish between fluid and elastic phases. The temporal deformation of the structure is described according to the backward characteristics which are employed to express the Cauchy stress of a two-parameter hyperelastic Mooney-Rivlin material. This model is particularly adapted to elastomeric materials undergoing large deformations, see figure 12 .

7.4. Overset grids

One of the difficulties in the simulation of a fluid flow problem is the representation of the computational domain with a static mesh. As a matter of fact, not only the geometry could be particularly complex in itself, but it could change during the simulation and this necessary involves an *in itinere* geometrical adaptation of the mesh, with a consequent high computational cost. One of the ways to overcome this problem is to use multiple overlapping mesh blocks that together define a *Chimera* or *overset* grid. Once the different mesh blocks are generated, they are properly composed by the creation of holes (*hole cutting*) and, consequently,

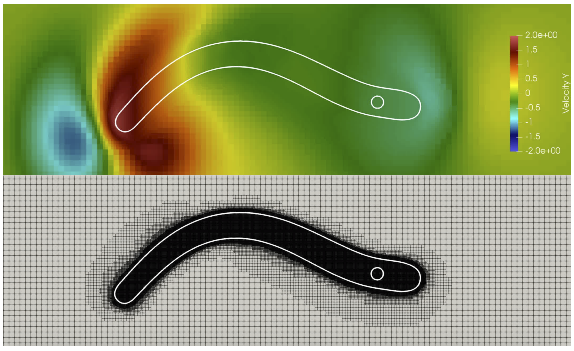


Figure 12. Y-component of the velocity for an oscillating elastomeric membrane actuated by a rigid holder at the tip, immersed in glycerin after 3 periods of oscillations. The criterion used for the dynamic AMR mesh is based on the level-set function.

an *overlapping zone* between two overlapping blocks is defined. Figure 13 shows a Chimera grid in the computational domain $[-\pi, \pi]^2$; in black there is the background mesh, in blue the foreground mesh. In particular, the foreground mesh can move and deform (consequently, the hole in the background mesh can change its configuration). The overlapping zone is necessary for the the communication and data transfer from one mesh to another. These operations are possible through an appropriate definition of local stencils of cells, both within and at the border of the individual blocks.
The Navier-Stokes equations for incompressible flows are going to be approximated through a projection method (*Chorin-Temam*), for this reason we have studied two Finite Volume (FV) solvers, for the pure diffusive equation and the unsteady convective-diffusive equation, on Chimera configurations. The first numerical experiments were conducted on 2D problems. The order of convergence of the error of the mismatch between the exact solution and its FV approximation in L^∞- and L^2-norms is 2.

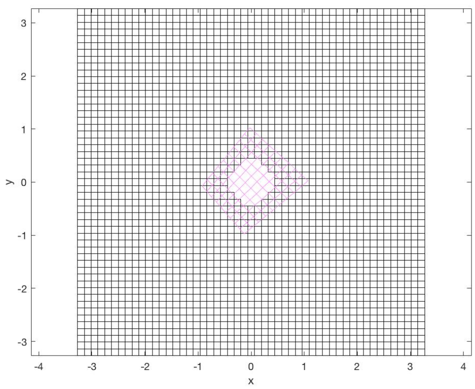


Figure 13. A Chimera grid configuration for the computational domain $[-\pi, \pi]^2$.

7.5. Collective propulsion: collaboration with ONERA

Motivated by recent studies and the locomotion of animal groups for robotics, we investigated the influence of hydrodynamic interactions on the collective propulsion of flapping wings. We studied the horizontal locomotion of an infinite array of flapping wings separated by a constant gap using unsteady non-linear simulations. Two control parameters were explored: the flapping frequency and the gap between the wings. Results obtained for different gaps at a fixed frequency are shown in Figure 14 . We first observe that for a very large spacing between the wings — greater than 20 times the chord of a wing — the interaction effects are no longer present (Figure 14 (b)) and the average speed of the system tends to the speed of a single wing. For lower gaps, the average speed may become lower or higher than that of a single wing. For certain gaps, one can find two different stable solutions: one at higher propulsion speed and the other lower than a single wing. This phenomenon has already been observed for a fixed spacing and different frequencies of movement. The stability of these solutions is linked to the interaction between the vortex wake generated by the previous wings and the vortex ejected at the leading or trailing edge of the considered wing (Figure 14 (a)). We remark that propulsive efficiency is higher for the collective case both in faster and slower solutions. Understanding the key mechanisms responsible for the stable solutions will provide directions to control strategies aiming to optimize the wing horizontal speed.

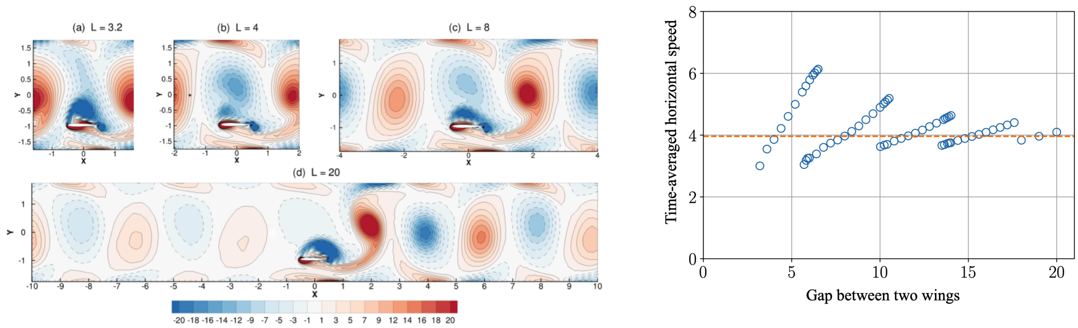


Figure 14. Vorticity contours (a) and time-averaged horizontal speed (b) for a flapping wing interacting in an infinite array. In (b) the average speed of a non interacting flapping wing is represented by a dashed orange line.

7.6. Automatic registration for model reduction

As part of the ongoing team effort on ROMs, we work on the development of automatic registration procedures for model reduction. In computer vision and pattern recognition, registration refers to the process of finding a spatial transformation that aligns two datasets; in our work, registration refers to the process of finding a parametric transformation that improves the linear compressibility of a given parametric manifold. For advection-dominated problems, registration is motivated by the inadequacy of linear approximation spaces due to the presence of parameter-dependent boundary layers and travelling waves.

In [48], we proposed and analysed a computational procedure for stationary PDEs and investigated performance for two-dimensional model problems. In Figure 15 , we show slices of the parametric solution for three different parameters before (cf. Left) and after (cf. Right) registration: we observe that the registration procedure is able to dramatically reduce the sensitivity of the solution to the parameter value μ. In Figure 16 , we show the behaviour of the normalised POD eigenvalues (cf. Left) and of the relative L^2 error of the corresponding POD-Galerkin ROM (cf. Right) for an advection-reaction problem: also in this case, the approach is able to improve the approximation properties of linear approximation spaces and ultimately simplify the reduction task.

We aim to extend the approach to a broad class of non-linear steady and unsteady PDEs: in October 2019, we funded a 16-month postdoc to work on the reduction of hyperbolic systems of PDEs. We are also collaborating with EDF (departments PERICLES and LNHE) to extend the approach to the Saint-Venant (shallow water) equations.

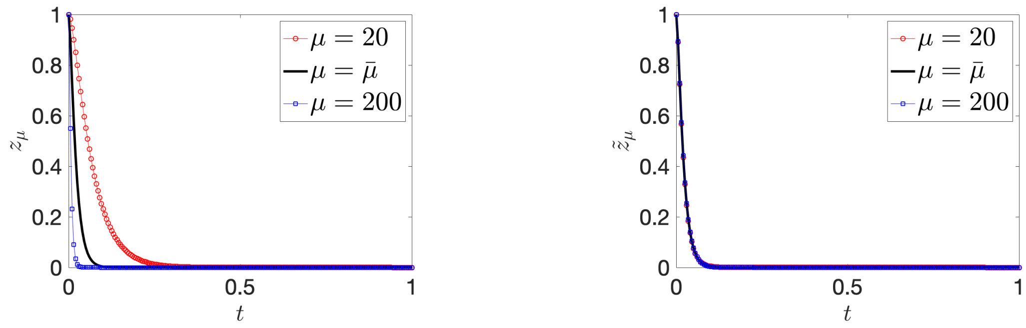


Figure 15. automatic registration for model reduction. Registration of a boundary layer ($\overline{\mu} = \sqrt{20 \cdot 200}$).

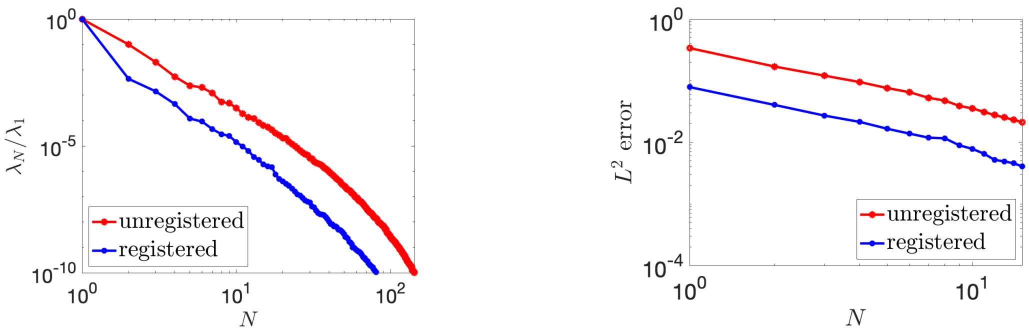


Figure 16. automatic registration for model reduction. Registration of a parameterized advection-reaction problem.

7.7. Modeling and numerical simulation of ellipsoidal particle-laden flows and self propelled swimmers in a porous enclosure

Despite being relevant in many natural and industrial processes, suspensions of non-spherical particles have been largely under-investigated compared to the extensive analyses made on the gravity-driven motions of spherical particles. One of the main reasons for this disparity is the difficulty of accurately correcting the short-range hydrodynamic forces and torques acting on complex particles. These effects, also known as lubrication, are essential to the suspension of the particles and are usually poorly captured by direct numerical simulation of particle-laden flows. We have proposed a partitioned VP-DEM (Volume Penalization method - Discrete Element Method) solver which estimates the unresolved hydrodynamic forces and torques. Corrections are made locally on the surface of the interacting particles without any assumption on the particle global geometry.

This is an extension of our previous work [39]. Numerical validations have been made using ellipsoidal particles immersed in an incompressible Navier-Stokes flow.

Self organization of groups of several swimmers is of interest in biological applications. One of the main question is to determine if the possible organization comes from an uncontrolled or a controlled swimming behavior. This work has been motivated by the recent studies of Hamid Kellay (LOMA). Hamid Kellay has presented his results during a small workshop we organized earlier this year between members of the Memphis team (modeling and numerical methods), the MRGM (experimental zebra-fishes swimming), the LOMA (interaction between self-propelled particles) and the ONERA (flapping wings).

The collision model developed in the previous section has been developed for concave interactions like sphere-sphere or in the limit of sphere-plane wall. For non concave interactions, we have derived a simple approximation considering locally convexity as being a plane wall. We have performed numerical simulations of the interaction of several self propelled swimmers in a porous enclosure (see figure 17). Fishes are organized in small groups that are able to put into motion the enclosure. This behavior is similar to the one observed in the experimental set-up of Hamid Kellay.

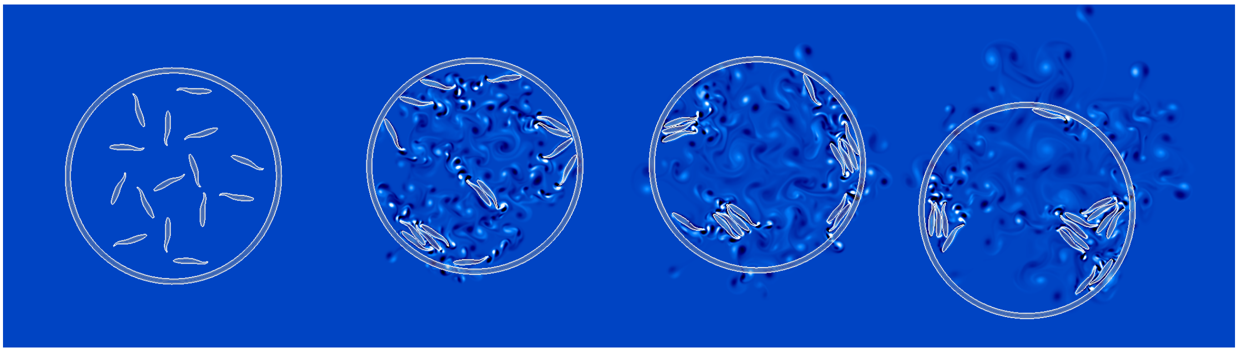


Figure 17. Organization of small self propelled fish groups in a porous enclosure (time evolution is in the usual reading direction). Colormap is the vorticity field.

MEPHYSTO Team

5. New Results

5.1. Traveling waves for some nonlocal 1D Gross-Pitaevskii equations with nonzero conditions at infinity

The nonlocal Gross-Pitaevskii equation is a model that appears naturally in several areas of quantum physics, for instance in the description of superfluids and in optics when dealing with thermo-optic materials because the thermal nonlinearity is usually highly nonlocal. A. de Laire and P. Mennuni have considered a nonlocal family of Gross–Pitaevskii equations in dimension one, and they have provided in [27] conditions on the nonlocal interaction such that there is a branch of traveling waves solutions with nonvanishing conditions at infinity. Moreover, they showed that the branch is orbitally stable. In this manner, this result generalizes known properties for the contact interaction given by a Dirac delta function. Their proof relies on the minimization of the energy at fixed momentum.

5.2. Numerical simulation of traveling waves for some nonlocal Gross-Pitaevskii equations with nonzero conditions at infinity in dimensions 1 and 2

As a follow-up of the previous result, P. Mennuni and G. Dujardin carried out numerical simulations of traveling waves for some nonlocal nonlinear Gross-Pitaevskii equations with nonzero conditions at infinity in dimensions 1 and 2. Using a numerical analogue of the minimization of the energy at fixed momentum, they used gradient methods with nonuniform fast Fourier transforms (to deal with the nonlocal terms numerically) to carry out significant numerical simulations to illustrate numerically the theoretical results and to discuss the hypotheses numerically. These results can be found in P. Mennuni's PhD manuscript [10].

5.3. The cubic Schrödinger regime of the Landau-Lifshitz equation with a strong easy-axis anisotropy

It is well-known that the dynamics of biaxial ferromagnets with a strong easy-axis anisotropy is essentially governed by the cubic Schrödinger equation. A. de Laire and P. Gravejat provided in [26] 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 cubic Schrödinger equation in the regime of an easy-axis anisotropy. This result holds for solutions to the Landau–Lifshitz equation in high order Sobolev spaces. By introducing high order energy quantities with good symmetrization properties, they derived the convergence from the consistency of the Landau–Lifshitz equation with the Sine-Gordon equation by using well-tailored energy estimates.

In this regime, they additionally classified the one-dimensional solitons of the Landau-Lifshitz equation and quantified their convergence towards the solitons of the one-dimensional cubic Schrödinger equation.

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

A. de Laire and S. Gutierrez established in [22] 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 step function and established their stability. They also showed the existence of multiple solutions if the damping is strong enough.

5.5. Microscopic derivation of moving interfaces problems

In [15], M. Simon and her coauthors derive the porous medium equation from an interacting particle system which belongs to the family of kinetically constrained lattice gases. It was already proved in the literature that the macroscopic density profile is governed by the porous medium equation for initial densities uniformly bounded away from 0 and 1. Here we consider the more general case where the density can take those extreme values. The solutions display a richer behavior, like moving interfaces, finite speed of propagation and breaking of regularity. Since standard techniques cannot be straightforwardly applied, we present a way to generalize the relative entropy method, by involving approximations of solutions to the hydrodynamic equation, instead of exact solutions.

In [16], M. Simon and her coauthors study the hydrodynamic limit for a similar one-dimensional exclusion process but with an even more restricting dynamical constraint: this process with degenerate jump rates admits transient states, which it eventually leaves to reach an ergodic component if the initial macroscopic density is larger than a critical value, or one of its absorbing states otherwise. They show that, for initial profiles smooth enough and uniformly larger than the critical density, the macroscopic density profile evolves under the diffusive time scaling according to a fast diffusion equation. The first step in the proof is to show that the system typically reaches an ergodic component in subdiffusive time.

These two macroscopic behaviors belong to the class of moving interfaces problems, which are particularly hard to derive from the microscopic point of view.

5.6. Towards the weak KPE universality conjecture

In [32], P. Gonçalves, N. Perkowski and M. Simon derive the KPZ equation with boundary conditions, from an interacting particle system in contact with stochastic reservoirs, and they legitimate the choice done at the macroscopic level for the KPZ equation from the microscopic description of the system. This is more subtle than expected, because the boundary conditions do not behave canonically. The main challenge is to clarify the link between the macroscopic boundary effects and their atomic description.

5.7. Joule effect in chains of oscillators

In physics, the rotor chain has been investigated as an example of a system with two conserved quantities (angular momentum and energy), for which the thermal conductivity is finite (and therefore energy diffuses). Numerics shows an unexpected behaviour of the chain when the latter is connected at the boundaries to two thermostats, and a mechanical force imposes an average angular momentum at one boundary: the stationary temperature profile coincides with the values of the thermostats, but in the middle of the chain it raises to a much higher value. This behaviour is related to the presence of two conserved quantities and is sometimes referred to as Joule effect. Since the rotor model is too difficult to be treated analytically, T. Komorowski, S. Olla and M. Simon investigate in [25] the harmonic chain of oscillators, perturbed with a stochastic noise, which makes the heat transport diffusive, namely: the noise destroys the conservation law of the total momentum, but keeps the other two conservation laws (energy and stretch) intact. The boundaries of the chain are connected to two Langevin thermostats and an external force acting on one boundary puts the system in a non-equilibrium stationary state. The authors rigorously derive the Joule effect for a particular value of the noise intensity.

5.8. Quantum optics

In [18], S. De Bièvre and his co-authors introduce a new measure of the nonclassicality of the quantum states of an optical field, the so-called “ordering sensitivity” of the state, that measures the fluctuations of its Wigner function. This work is prolonged in two subsequent papers. In [24], S. De Bièvre and the same co-authors investigate a new class of quantum states they call the “Thermal Difference States” that can be generated by parametric down conversion. They investigate in particular the degree to which such states are nonclassical. In [34], S. De Bièvre and his postdoc A. Hertz, re-interpret the ordering sensitivity in terms of another physical property of the quantum states of an optical field, namely their quadrature coherence scale. It is shown in particular that a large such coherence scale is responsible for very fast environmental decoherence of the state.

5.9. Orbital stability

In [19], S. De Bièvre and S. Rota Nodari consider 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. They prove a persistence result for such relative equilibria, present a generalization of the Vakhitov-Kolokolov slope condition to this higher dimensional setting, and show how it allows to prove the local coercivity of the Lyapunov function, which in turn implies orbital stability. The method is applied to study the orbital stability of relative equilibria of nonlinear Schrödinger and Manakov equations. A comparison of their approach to the one by Grillakis-Shatah-Strauss is provided.

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

In the research direction exposed in Section 3.3 , G. Dujardin and his coauthors proposed and studied in [21] 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 for the very first time hypocoercive methods to the discrete level.

5.11. 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.

5.12. High order linearly implicit methods for evolution problems

In [31], I. Lacroix and G. Dujardin have developed a new class of numerical integration methods for evolution problems. This class contains methods of arbitrarily high order that only require the solution of a linear system per time step. For evolution ODEs (Cauchy problems), they give a constructive proof of existence for such arbitrarily high order methods. For evolution PDEs, they demonstrate numerically that these new methods can outperform high order methods from the literature on several test cases.

5.13. CLT for Circular beta-Ensembles at High Temperature

In [33], A. Hardy and G. Lambert have obtained a central limit theorem for the 2D Coulomb gas particle system constrained on a circle in the high temperature regime. An interesting feature is that the limiting variance interpolates between the Lebesgue L^2 norm, corresponding to the infinite temperature setting, and the Sobolev $H^{1/2}$ seminorm, corresponding to the zero temperature regime.

5.14. DLR equations and rigidity for the Sine-β process

The work [20] by A. Hardy and his collaborators, recently accepted for publication in Communications on Pure and Applied Mathematics, provides a "statistical physics" description of the sine-β process by means of Dobroshin-Lanford-Ruelle (DLR) equations. This basically allows to give a meaning to "the natural infinite configurations process on the real line in the 2D Coulomb interaction", provided there is a unique solution to the DLR equation which turns out to be true in this setting.

MINGUS Project-Team

6. New Results

6.1. New Results

Analysis of PDEs and SPDEs

In [17], we prove the nonlinear instability of inhomogeneous steady states solutions to the Hamiltonian Mean Field (HMF) model. We first study the linear instability of this model under a simple criterion by adapting the techniques developed by the authors recently. In a second part, we extend to the inhomogeneous case some techniques developed by the authors recently and prove a nonlinear instability result under the same criterion.

In [24], we consider the non linear wave equation (NLW) on the d-dimensional torus with a smooth nonlinearity of order at least two at the origin. We prove that, for almost any mass, small and smooth solutions of high Sobolev indices are stable up to arbitrary long times with respect to the size of the initial data. To prove this result we use a normal form transformation decomposing the dynamics into low and high frequencies with weak interactions. While the low part of the dynamics can be put under classical Birkhoff normal form, the high modes evolve according to a time dependent linear Hamiltonian system. We then control the global dynamics by using polynomial growth estimates for high modes and the preservation of Sobolev norms for the low modes. Our general strategy applies to any semi-linear Hamiltonian PDEs whose linear frequencies satisfy a very general non resonance condition. The (NLW) equation on a torus is a good example since the standard Birkhoff normal form applies only when $d = 1$ while our strategy applies in any dimension.

In [20], we study semigroups generated by accretive non-selfadjoint quadratic differential operators. We give a description of the polar decomposition of the associated evolution operators as products of a selfadjoint operator and a unitary operator. The selfadjoint parts turn out to be also evolution operators generated by time-dependent real-valued quadratic forms that are studied in details. As a byproduct of this decomposition, we give a geometric description of the regularizing properties of semigroups generated by accretive non-selfadjoint quadratic operators. Finally, by using the interpolation theory, we take advantage of this smoothing effect to establish subelliptic estimates enjoyed by quadratic operators.

In [16], 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.

In [25], we study the Boltzmann equation with external forces, not necessarily deriving from a potential, in the incompressible Navier-Stokes perturbative regime. On the torus, we establish local-in-time, for any time, Cauchy theories that are independent of the Knudsen number in Sobolev spaces. The existence is proved around a time-dependent Maxwellian that behaves like the global equilibrium both as time grows and as the Knudsen number decreases. We combine hypocoercive properties of linearized Boltzmann operators with linearization around a time-dependent Maxwellian that catches the fluctuations of the characteristics trajectories due to the presence of the force. This uniform theory is sufficiently robust to derive the incompressible Navier-Stokes-Fourier system with an external force from the Boltzmann equation. Neither smallness, nor time-decaying assumption is required for the external force, nor a gradient form, and we deal with general hard potential and cutoff Boltzmann kernels. As a by-product the latest general theories for unit Knudsen number when the force is sufficiently small and decays in time are recovered.

In [15], we show how the methods recently applied by Debussche and Weber to solve the stochastic nonlinear Schrödinger equation on $\mathbb{T}^2$ can be enhanced to yield solutions on $\mathbb{R}^2$ if the non-linearity is weak enough. We prove that the solutions remains localized on compact time intervals which allows us to apply energy methods on the full space.

In [2], we provide in this work a local in time well-posedness result for a quasilinear generalized parabolic Anderson model in dimension two $\partial_t u + \Delta\Pi(u) = g(u)\xi$. The key idea of our approach is a simple transformation of the equation which allows to treat the problem as a semilinear problem. The analysis is done within the setting of paracontrolled calculus.

In [30], we consider the Burgers equation on $H = L^2(0,1)$ perturbed by white noise and the corresponding transition semigroup $P_t D\varphi$. We prove a new formula for $PtD\varphi$ (where $\varphi : H \to \mathbb{R}$ is bounded and Borel) which depends on φ but not on its derivative. Then we deduce some consequences for the invariant measure ν of P_t as its Fomin differentiability and an integration by parts formula which generalises the classical one for gaussian measures.

In [9], we deal with the validity of a large deviation principle for the two-dimensional Navier-Stokes equation, with periodic boundary conditions, perturbed by a Gaussian random forcing. We are here interested in the regime where both the strength of the noise and its correlation are vanishing, on a length scale ε and $\delta(\varepsilon)$, respectively, with $0 < \varepsilon, \delta(\varepsilon) << 1$. Depending on the relationship between ε and $\delta(\varepsilon)$ we will prove the validity of the large deviation principle in different functional spaces.

In [30], the authors consider the transition semigroup P_t of the Φ^4_2 stochastic quantisation on the torus $\mathbb{T}^2$ and prove the following new estimate

$$|DP_t\varphi(x)\cdot h| \leq ct^{-\beta}|h|_{C^{-s}}\|\varphi\|_0(1+|x|_{C^{-s}})^\gamma,$$

for some α, β, γ, s positive. Thanks to this estimate, we show that cylindrical functions are a core for the corresponding Kolmogorov equation. Some consequences of this fact are discussed in a final remark.

In [32], we consider a particle system with a mean-field-type interaction perturbed by some common and individual noises. When the interacting kernels are sublinear and only locally Lipschitz-continuous, relying on arguments regarding the tightness of random measures in Wasserstein spaces, we are able to construct a weak solution of the corresponding limiting SPDE. In a setup where the diffusion coefficient on the environmental noise is bounded, this weak convergence can be turned into a strong $L^p(\Omega)$ convergence and the propagation of chaos for the particle system can be established. The systems considered include perturbations of the Cucker-Smale model for collective motion.

Numerical schemes

In [7], the asymptotic behavior of the solutions of the second order linearized Vlasov-Poisson system around homogeneous equilibria is derived. It provides a fine description of some nonlinear and multidimensional phenomena such as the existence of Best frequencies. Numerical results for the $1D \times 1D$ and $2D \times 2D$ Vlasov-Poisson system illustrate the effectiveness of this approach.

In [6], 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.

In [4], 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.

The efficient numerical solution of many kinetic models in plasma physics is impeded by the stiffness of these systems. Exponential integrators are attractive in this context as they remove the CFL condition induced by the linear part of the system, which in practice is often the most stringent stability constraint. In the literature, these schemes have been found to perform well, e.g., for drift-kinetic problems. Despite their overall efficiency and their many favorable properties, most of the commonly used exponential integrators behave rather erratically in terms of the allowed time step size in some situations. This severely limits their utility and robustness. Our goal in [29] is to explain the observed behavior and suggest exponential methods that do not suffer from the stated deficiencies. To accomplish this we study the stability of exponential integrators for a linearized problem. This analysis shows that classic exponential integrators exhibit severe deficiencies in that regard. Based on the analysis conducted we propose to use Lawson methods, which can be shown not to suffer from the same stability issues. We confirm these results and demonstrate the efficiency of Lawson methods by performing numerical simulations for both the Vlasov-Poisson system and a drift-kinetic model of a ion temperature gradient instability.

In [18], a bracket structure is proposed for the laser-plasma interaction model introduced in the physical literature, and it is proved by direct calculations that the bracket is Poisson which satisfies the Jacobi identity. Then splitting methods in time are proposed based on the Poisson structure. For the quasi- relativistic case, the Hamiltonian splitting leads to three subsystems which can be solved exactly. The conservative splitting is proposed for the fully relativistic case, and three one-dimensional conservative subsystems are obtained. Combined with the splittings in time, in phase space discretization we use the Fourier spectral and finite volume methods. It is proved that the discrete charge and discrete Poisson equation are conserved by our numerical schemes. Numerically, some numerical experiments are conducted to verify good conservations for the charge, energy and Poisson equation.

In [26], the recent advances about the construction of a Trefftz Discontinuous Galerkin (TDG) method to a class of Friedrichs systems coming from linear transport with relaxation are presented in a comprehensive setting. Application to the $2DP_N$ model are discussed, together with the derivation of new high order convergence estimates and new numerical results for the P_1 and P_3 models. More numerical results in dimension 2 illustrate the theoretical properties.

In [8], we are concerned with a formulation of Magnus and Floquet-Magnus expansions for general nonlinear differential equations. To this aim, we introduce suitable continuous variable transformations generated by operators. As an application of the simple formulas so-obtained, we explicitly compute the first terms of the Floquet-Magnus expansion for the Van der Pol oscillator and the nonlinear Schrödinger equation on the torus.

The article [11] 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. We illustrate the properties of our methods with simulations.

In [10], we 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.

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 [13] is a first step towards the resolution of these difficulties. In particular, we 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.

In [12], 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.

In [1], 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.

In [22], a splitting strategy is introduced to approximate two-dimensional rotation motions. Unlike standard approaches based on directional splitting which usually lead to a wrong angular velocity and then to large error, the splitting studied here turns out to be exact in time. Combined with spectral methods, the so-obtained numerical method is able to capture the solution to the associated partial differential equation with a very high accuracy. A complete numerical analysis of this method is given in this work. Then, the method is used to design highly accurate time integrators for Vlasov type equations: the Vlasov-Maxwell system and the Vlasov-HMF model. Finally , several numerical illustrations and comparisons with methods from the literature are discussed.

In [23], some exact splittings are proposed for inhomogeneous quadratic differential equations including, for example, transport equations, kinetic equations, and Schrödinger type equations with a rotation term. In this work, these exact splittings are combined with pseudo-spectral methods in space to illustrate their high accuracy and efficiency.

In [14], 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 an 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 an asymptotically complexity diminishing scheme (ACDS) - 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.

In [5], we revisit the old problem of compact finite difference approximations of the homogeneous Dirichlet problem in dimension 1. We design a large and natural set of schemes of arbitrary high order, and we equip this set with an algebraic structure. We give some general criteria of convergence and we apply them to obtain two new results. On the one hand, we use Padé approximant theory to construct, for each given order of consistency, the most efficient schemes and we prove their convergence. On the other hand, we use diophantine approximation theory to prove that almost all of these schemes are convergent at the same rate as the consistency order, up to some logarithmic correction.

In [28], we introduce a new Monte Carlo method for solving the Boltzmann model of rarefied gas dynamics. The method works by reformulating the original problem through a micro-macro decomposition and successively in solving a suitable equation for the perturbation from the local thermodynamic equilibrium. This equation is then discretized by using unconditionally stable exponential schemes in time which project the solution over the corresponding equilibrium state when the time step is sent to infinity. The Monte Carlo method is designed on this time integration method and it only describes the perturbation from the final state. In this way, the number of samples diminishes during the time evolution of the solution and when the final equilibrium state is reached, the number of statistical samples becomes automatically zero. The resulting method is computationally less expensive as the solution approaches the equilibrium state as opposite to standard methods for kinetic equations which computational cost increases with the number of interactions. At the same time, the statistical error decreases as the system approaches the equilibrium state. In a last part, we show the behaviors of this new approach in comparison with standard Monte Carlo techniques and in comparison with spectral methods on different prototype problems.

In [27], we consider the three dimensional Vlasov equation with an inhomogeneous, varying direction, strong magnetic field. Whenever the magnetic field has constant intensity, the oscillations generated by the stiff term are periodic. The homogenized model is then derived and several state-of-the-art multiscale methods, in combination with the Particle-In-Cell discretisation, are proposed for solving the Vlasov-Poisson equation. Their accuracy as much as their computational cost remain essentially independent of the strength of the magnetic field. The proposed schemes thus allow large computational steps, while the full gyro-motion can be restored by a linear interpolation in time. In the linear case, extensions are introduced for general magnetic field (varying intensity and direction). Eventually, numerical experiments are exposed to illustrate the efficiency of the methods and some long-term simulations are presented.

MOKAPLAN Project-Team

5. New Results

5.1. An augmented Lagrangian approach to Wasserstein gradient flows and applications

Benamou, Jean-David and Carlier, Guillaume and Laborde, Maxime. In [2] : Taking advantage of the Benamou-Brenier dynamic formulation of optimal transport, we propose a convex formulation for each step of the JKO scheme for Wasserstein gradient flows which can be attacked by an augmented Lagrangian method which we call the ALG2-JKO scheme. We test the algorithm in particular on the porous medium equation. We also consider a semi implicit variant which enables us to treat nonlocal interactions as well as systems of interacting species. Regarding systems, we can also use the ALG2-JKO scheme for the simulation of crowd motion models with several species.

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

Benamou, Jean-David and Carlier, Guillaume and Marino, Simone Di and Nenna, Luca. In [18] : We propose an entropy minimization viewpoint on variational meanfield games with diffusion and quadratic Hamiltonian. We carefully analyze the time-discretization of such problems, establish Γ-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.

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

Benamou, Jean-David and Duval, Vincent. In [3] : We propose an adaptation of the MA-LBR scheme to the Monge-Ampère equation with second boundary value condition, provided the target is a convex set. This yields a fast adaptive method to numerically solve the Optimal Transport problem between two absolutely continuous measures, the second of which has convex support. The proposed numerical method actually captures a specific Brenier solution which is minimal in some sense. We prove the convergence of the method as the grid stepsize vanishes and we show with numerical experiments that it is able to reproduce subtle properties of the Optimal Transport problem

We propose an entropy minimization viewpoint on variational meanfield games with diffusion and quadratic Hamiltonian. We carefully analyze the time-discretization of such problems, establish Γ-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.

5.4. Sparse analysis methods for Mesoscale Convective Systems (MCS)

Jean-Baptiste Courbot, Vincent Duval and Bernard Legras. In [20] : Mesoscale Convective Systems (MCS) are organized cloud systems which constitute the major part of the high cloud cover in the tropical region, where they can reach sizes of up to 1000 km in diameter. Under some favorable circumstances, they can eventually organize as tropical cyclones. Due to the complexity and the huge amount of available information, there is a need for an automatic tool able to detect and keep track of MCS in time series of these images. In [20] we have proposed a new method for the tracking of those cloud systems in infrared satellite images.

5.5. Pareto optimality with transport costs

Bruno Nazaret, Xavier Bacon, Guillaume Carlier, Thomas Gallouët. Arrived in September 2019, B. Nazaret, with his Phd student X. Bacon, has started a collaboration with G. Carlier on a Pareto optimality model with transport costs. He also has initiated a study with T.O. Gallouët of of a first order proximal scheme for densities on Euclidean half-spaces, with the additional feature that the boundary moves while the mass still remains constant along the time.

5.6. An epigraphical approach to the representer theorem

Duval, Vincent. In [22] : Describing the solutions of inverse problems arising in signal or image processing is an important issue both for theoretical and numerical purposes. In [22], we have proposed a principle which describes the solutions to convex variational problems involving a finite number of measurements. We discuss its optimality on various problems concerning the recovery of Radon measures.

5.7. Approximate Optimal Designs for Multivariate Polynomial Regression

De Castro, Yohann et al. In [8] : 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. Describing the solutions of inverse problems arising

5.8. Sparse Recovery from Extreme Eigenvalues Deviation Inequalities

De Castro, Yohann et al. In [7] : This article provides a new toolbox to derive sparse recovery guarantees. It is ususally referred to as “stable and robust sparse regression” (SRSR) ’ from deviations on extreme singular values or extreme eigenvalues obtained in Random Matrix Theory. This work is based on Restricted Isometry Constants (RICs) which are a pivotal notion in Compressed Sensing and High-Dimensional Statistics as these constants finely assess how a linear operator is conditioned on the set of sparse vectors and hence how it performs in SRSR. While it is an open problem to construct deterministic matrices with apposite RICs, one can prove that such matrices exist using random matrices models. In this paper, we show upper bounds on RICs for Gaussian and Rademacher matrices using state-of-the-art deviation estimates on their extreme eigenvalues. This allows us to derive a lower bound on the probability of getting SRSR. One benefit of this paper is a direct and explicit derivation of upper bounds on RICs and lower bounds on SRSR from deviations on the extreme eigenvalues given by Random Matrix theory.

5.9. Some new Stein operators for product distributions

Mijoule G. et al. In [12] : We provide a general result for finding Stein operators for the product of two independent random variables whose Stein operators satisfy a certain assumption, extending a recent result of Gaunt, R. E., Mijoule, G. and Swan. This framework applies to non-centered normal and non-centered gamma random variables, as well as a general sub-family of the variance-gamma distributions. Curiously, there is an increase in complexity in the Stein operators for products of independent normals as one moves, for example, from centered to non-centered normals. As applications, we give a simple derivation of the characteristic function of the product of independent normals, and provide insight into why the probability density function of this distribution is much more complicated in the non-centered case than the centered case.

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

C. Cancès, T. O. Gallouët, M. Laborde, L. Monsaingeon. In [6]: the Wasserstein gradient flow structure of the PDE system governing multiphase flows in porous media was recently highlighted in [68]. 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 [2]. The numerical results are compared to a classical upstream mobility Finite Volume scheme, for which strong stability properties can be established.

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

T. O. Gallouët, M. Laborde, L. Monsaingeon. In [10] 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.

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

C .Cancès, T. O. Gallouët, G. Todeschi. We propose a variational finite volume scheme to approximate the solutions to Wasserstein gradient flows. The time discretization is based on an implicit linearization of the Wasserstein distance expressed thanks to Benamou-Brenier formula, whereas space discretization relies on upstream mobility two-point flux approximation finite volumes. Our scheme is based on a first discretize then optimize approach in order to preserve the variational structure of the continuous model at the discrete level. Our scheme can be applied to a wide range of energies, guarantees non-negativity of the discrete solutions as well as decay of the energy. We show that our scheme admits a unique solution whatever the convex energy involved in the continuous problem , and we prove its convergence in the case of the linear Fokker-Planck equation with positive initial density. Numerical illustrations show that it is first order accurate in both time and space, and robust with respect to both the energy and the initial profile.

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

T. O. Gallouët, A. Natale, F-X. Vialard. In [11] : 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.

5.14. Metric completion of $\mathrm{Diff}([0,1])$ with the right-invariant H^1 metric

S. di Marino, A. Natale, R. Tahraoui, F-X. Vialard. In [21]: We consider the group of smooth increasing diffeomorphisms Diff on the unit interval endowed with the right-invariant H1 metric. We compute the metric completion of this space which appears to be the space of increasing maps of the unit interval with boundary conditions at 0 and 1. We compute the lower-semicontinuous envelope associated with the length minimizing geodesic variational problem. We discuss the Eulerian and Lagrangian formulation of this relaxation and we show that smooth solutions of the EPDiff equation are length minimizing for short times.

5.15. Embedding Camassa-Holm equations in incompressible Euler

A. Natale, F-X. Vialard. In [13] : In this article, we show how to embed the so-called CH2 equations into the geodesic flow of the $H(\mathrm{div})$ metric in 2D, which, itself, can be embedded in the incompressible Euler equation of a non compact Riemannian manifold. The method consists in embedding the incompressible Euler equation with a potential term coming from classical mechanics into incompressible Euler of a manifold and seeing the CH2 equation as a particular case of such fluid dynamic equation.

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

J-D. Benamou, T. O. Gallouët, F-X. Vialard. In [4] : On the space of probability densities, we extend 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.

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. 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 has been accepted for publication in 2019.

6.1.3. Stability and asymptotic properties of the linearized Hydrodynamic Drude model

Participants: Serge Nicaise [Université de Valenciennes], Claire Scheid.

We go a step further toward a better understanding of the fundamental properties of the linearized hydrodynamical model studied in the PhD of Nikolai Schmitt [16]. This model is especially relevant for small nanoplasmonic structures (below 10nm). Using a hydrodynamical description of the electron cloud, both retardation effects and non local spatial response are taken into account. This results in a coupled PDE system for which we study the linear response. In [45] (submitted, under revision), we concentrate on establishing well posedness results combined to a theoretical and numerical stability analysis. We especially prove polynomial stability and provide optimal energy decay rate. Finally, we investigate the question of numerical stability of several explicit time integration strategies combined to a Discontinuous Galerkin spatial discretization.

6.1.4. Toward thermoplasmonics

Participants: Yves d'Angelo, 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.

6.1.5. Corner effects in nanoplasmonics

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

In this work, we study nanoplasmonic structures with corners (typically a diedral/triangular structure); a situation that raises a lot of issues. We focus on a lossles Drude dispersion model and propose to investigate the range of validity of the amplitude limit principle. The latter predicts the asymptotic harmonic regime of a structure that is monochromatically illuminated, which makes a frequency domain approach relevant. However, in frequency domain, several well posedness problems arise due to the presence of corners (addressed in the PhD thesis of Camille Carvalho). This should impact the validity of the limit amplitude principle and has not yet been addressed in the literature in this precise setting. Here, we combine frequency-domain and time-domain viewpoints to give a numerical answer to this question in two dimensions. We show that the limit amplitude principle does not hold for whole interval of frequencies, that are explicited using the well-posedness analysis. This work is now being finalized.

6.1.6. 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.

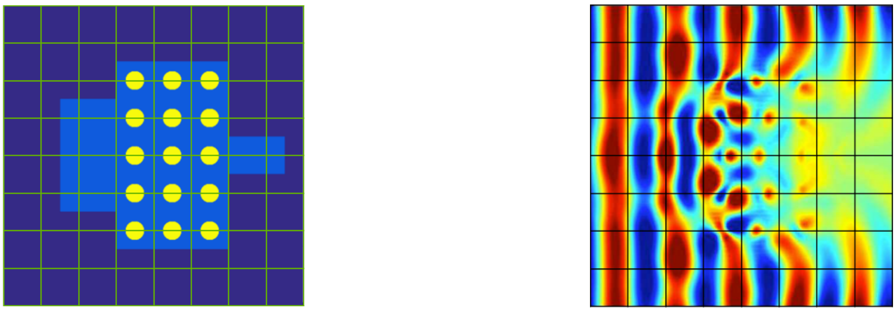


Figure 4. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

6.1.7. HDG methods for the time-domain Maxwell equations

Participants: Théophile Chaumont-Frelet, Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.

Hybridizable discontinuous Galerkin (HDG) methods have been investigated in the team since 2012. This family of method employs face-based degrees of freedom that can be viewed as a fine grain domain decomposition technique. We originally focused on frequency-domain applications, for which HDG methods enable the use of static condensation, leading to drastic reduction in computational time and memory consumption. More recently, we have investigated the use of HDG discretization to solve time-dependent problems. Specifically, in the context of the PhD thesis of Georges Nehmetallah, we focused on two particular aspects. On the one hand, HDG methods exhibit a superconvergence property that allows, by means of local postprocessing, to obtain new improved approximations of the unknowns. Our first contribution is to apply this methodology to time-dependent Maxwell's equations, where the post-processed approximation converges with order $k+1$ instead of k in the $H(curl)$-norm, when using polynomial of degree $k \geq 1$. The proposed method has been implemented for dealing with general 3D problems. Fig. 5 highlights the improved accuracy of the post-processed approximation on a cavity benchmark.

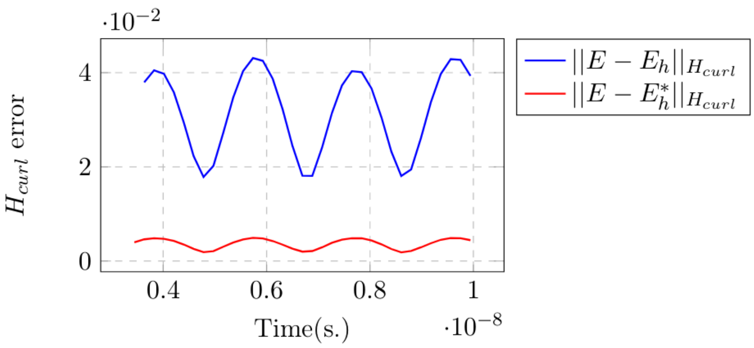


Figure 5. Time evolution of the $H(curl)$-error before and after postprocessing for P_2 interpolation and a fixed mesh constituted by 3072 elements

Another interesting aspect of the HDG method is that it can be conveniently employed to blend different time-integration schemes in different regions of the mesh. This is especially useful to efficiently handle locally refined space grids, that are required to take into account geometrical details. These ideas have already been explored for standard discontinuous Galerkin discretization in the context of the PhD thesis of Ludovic Moya [13], [14]. Here, we focused on HDG methods and we introduced a family of coupled implicit-explicit (IMEX) time integration methods for solving time-dependent Maxwell's equations. We established stability conditions that are independent of the size of the small elements in the mesh, and are only constrained by the coarse part. Numerical experiments on two-dimensional benchmarks illustrate the theory and the usefulness of the approach.

6.1.8. A posteriori error estimators

Participants: Théophile Chaumont-Frelet, Alexandre Ern [SERENA project-team], Patrick Vega, Martin Vohralík [SERENA project-team].

The development of *a posteriori* error estimators and is a new topic of interest for the team. Concerning *a posteriori* estimators, a collaboration with the SERENA project-team has been initiated. We mainly focus on a technique called equilibrated fluxes, which has the advantage to produce p-robust error estimators together with guaranteed error estimates. This means in particular that these estimators are particularly suited for high-order discretization schemes. Our first results deal with the Helmholtz equation, and have been recently submitted [39] and presented at the Enumath international conference [29]. Fig. 6 depicts the ability of the estimators to accurately describe the error distribution in a realistic application. Future works in this line will include the treatment of Maxwell's equations. The recently hired postdoctoral fellow Patrick Vega will actively participate in these developments.

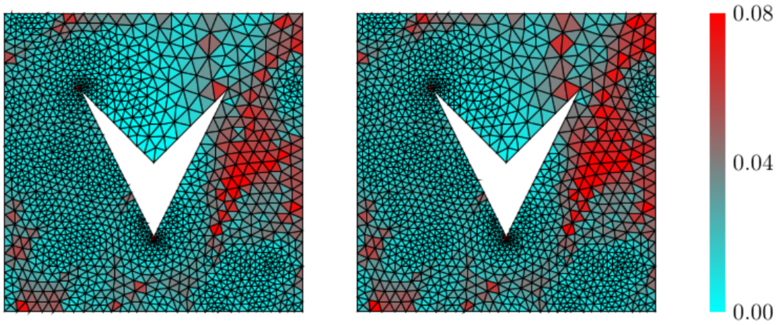
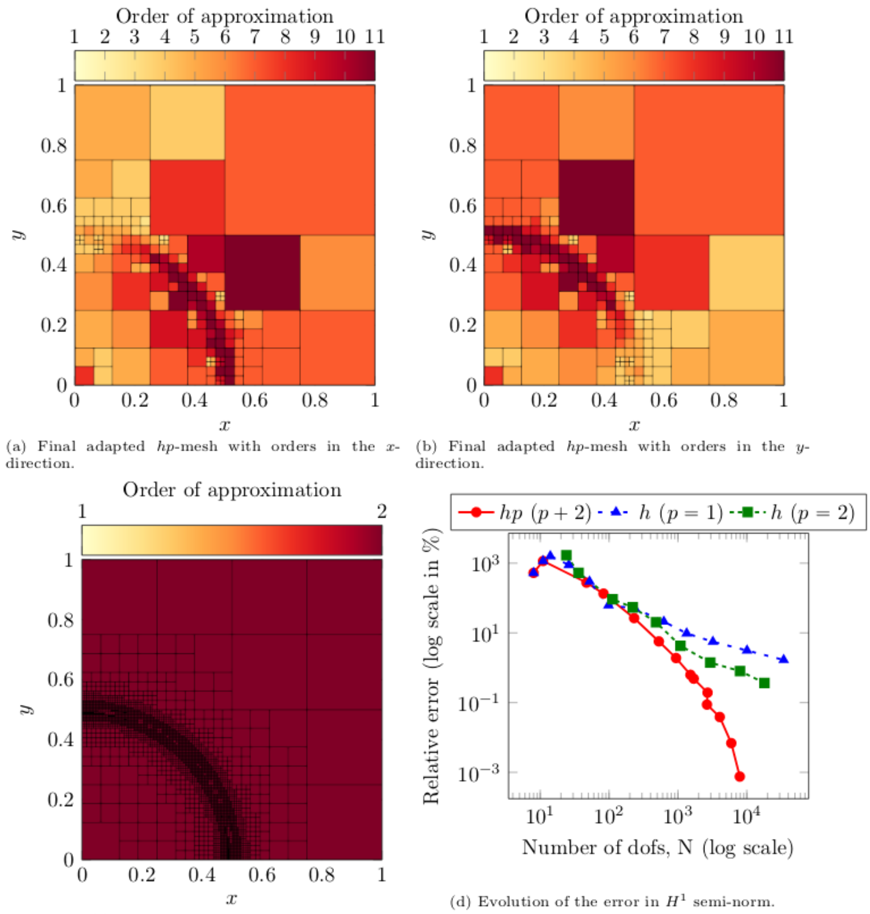


Figure 6. Estimators η_K (left) and elementwise errors $\|u - u_h\|_K$ (right) for a scattering problem discretized with $\mathcal{P}_3$ elements

6.1.9. hp-adaptivity

Participants: Théophile Chaumont-Frelet, David Pardo [Basque Center for Applied Mathematics, Bilbao, Spain].

Together with the development of a posteriori estimators, a novel activity in the team is the design of efficient hp-adpative strategy. In this regard, we propose a multi-level hierarchical data structure imposing Dirichlet nodes to manage the so-called hanging nodes. Our hp-adaptive strategy is based on performing quasi-optimal unrefinements. Taking advantage of the hierarchical structure of the basis functions both in terms of the element size h and the polynomial order of approximation p, we mark those with the lowest contributions to the energy of the solution and remove them. This straightforward unrefinement strategy does not require from a fine grid or complex data structures, making the algorithm flexible to many practical situations and existing implementations. Our first contribution has been recently submitted [42], and deals with the Poisson equation. Fig. 7 shows how the algorithm is able to correctly refine the computational grid to capture a shock wave.



(a) Final adapted hp-mesh with orders in the x-direction.
(b) Final adapted hp-mesh with orders in the y-direction.
(c) Final adapted h-mesh, $p = 2$.
(d) Evolution of the error in H^1 semi-norm.

Figure 7. Different hp-adptive strategies for capturing a shock wave

6.1.10. Multiscale methods for frequency-domain wave propagation

Participants: Théophile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri, Frédéric Valentin.

The design and analysis of multiscale methods for wave propagation is an important research line for team. The team actually mainly specializes in one family of multiscale methods, called multiscale hybrid-mixed (MHM). These developments started thanks to the close collaboration with Frédéric Valentin, who has recently been awarded an Inria international chair. Previous investigations in the context of this collaboration focused on time-dependent Maxwell's equations [10]. Recent efforts have been guided towards the realization of a MHM method for time-harmonic Maxwell's equations. We first focused on the Helmholtz equation, that modelizes the particular case of polarized waves. Our first results include the implementation of the method for two-dimensional problems as well as rigorous, frequency-explicit, stability and convergence analysis. These findings have recently been accepted for publication [40]. In the context of the internship of Zakaria Kassali, the method has been further adapted for the propagation of polarized waves in solar cells. Specifically, it is required in this case to take into account “quasi-periodic” boundary conditions that deserve a special treatment. We are currently undertaking further developments guided toward full three-dimensional Maxwell’s equations with the PhD of Zakaria Kassali, which started in November 2019.

6.2. High performance numerical computing

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

Participants: Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Théophile Chaumont-Frelet, Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

This work is undertaken in the context of PRACE 6IP project and aims at the development of scalable frequency-domain electromagnetic wave propagation solvers, in the framework of the DIOGENeS software suite. This solver 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 dispersive 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.

6.3. Applications

6.3.1. Inverse design of metasurfaces using statistical learning methods

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

Metasurfaces are flat optical nanocomponents, that are the basis of several more complicated optical devices. The optimization of their performance is thus a crucial concern, as they impact a wide range of applications. Yet, current design techniques are mostly based on *engineering knowledge*, and may potentially be improved by a rigorous analysis based on accurate simulation of Maxwell’s equations. The goal of this study is to optimize phase gradient metasurfaces by taking advantage of our fullwave high order Discontinuous Galerkin time-Domain solver implemented in DIOGENeS, coupled with two advanced optimization techniques based on statistical learning and evolutionary strategies. Our key findings are novel designs for Gan semiconductor phase gradient metasurfaces operating at visible wavelengths. Our numerical results reveal that rectangular and cylindrical nanopillar arrays can achieve more than respectively 88% and 85% of diffraction efficiency for TM polarization and both TM and TE polarization respectively, using only 150 fullwave simulations. To the best of our knowledge, this is the highest blazed diffraction efficiency reported so far at visible wavelength using such metasurface architectures. Fig. 8 depicts the superiority of the proposed statistical learning approaches over standard gradient-based optimization strategies. This work has been recently published [22].

6.3.2. Optimization of light-trapping in nanocone gratings

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

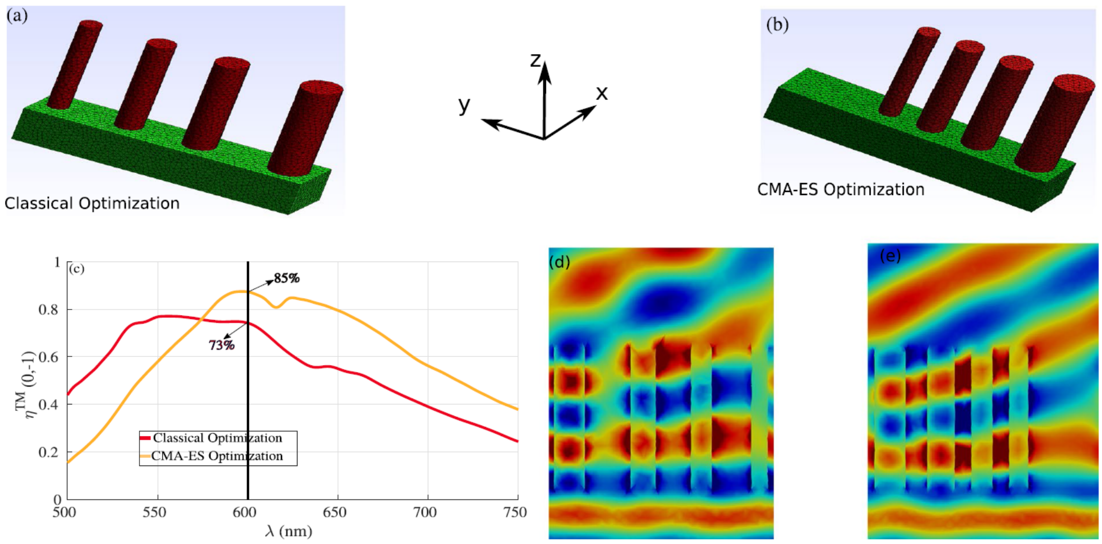


Figure 8. Comparison between the classical approach to phase gradient metasurface design and our optimized geometries for the cylindrical nanopillars with $h = 800$ nm. (a,b) The geometry obtained using the classical approach in which each nanopillar is optimized manually by changing the diameter and finally placed together in order to obtain the desired phase shift needed to maximize the light deflection for the first order mode at $\lambda = 600$ nm with period 1500 nm in y-direction. (c) Results obtained using the CMA-ES for the cylindrical nanopillars (see Table 3) for the corresponding parameters. (c) Comparison between the deflection efficiency for the first order mode obtained using the classical (red curve) and the CMA-ES (orange curve). (d,e) Represent field maps of $Re(E_y)$ obtained using the classical optimization design and the CMA-ES results, respectively

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 [60]. In the present study, we adopt the nanocone grating considered in [60]. This structure contains a crystalline silicon thin film with nanocone gratings also made of silicon. The circular 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. We use two efficient global optimization techniques based on statistical learning to adpat the geometrical characteristics of the nanocones in order the maximize the light absorption properties of this type of solr cells.

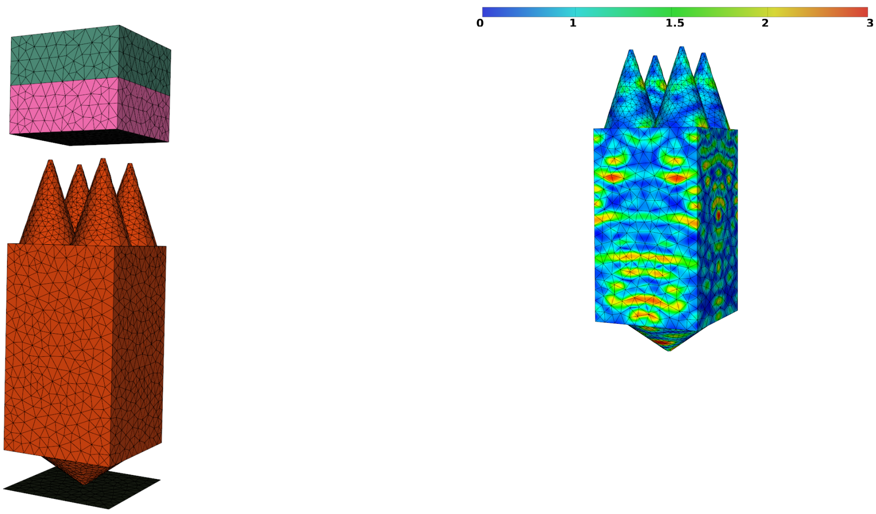


Figure 9. Simulation of light trapping in a solar cell based on nanocone gratings. Geometrical model (left) and contour lines of the module of the DFT of $\mathbf{E}$ *for a wavelength* $\lambda = 857$ *nm (right).*

6.3.3. Influence of spatial dispersion on surface plasmons and grating couplers

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

Recent experiments have shown that spatial dispersion may have a conspicuous impact on the response of plasmonic structures. This suggests that in some cases the Drude model should be replaced by more advanced descriptions that take spatial dispersion into account, like the hydrodynamic model. Here we show that nonlocality in the metallic response affects surface plasmons propagating at the interface between a metal and a dielectric with high permittivity. As a direct consequence, any nanoparticle with a radius larger than 20 nm can be expected to be sensitive to spatial dispersion whatever its size. The same behavior is expected for a simple metallic grating allowing the excitation of surface plasmons, just as in Woods famous experiment. Finally, we carefully set up a procedure to measure the signature of spatial dispersion precisely, leading the way for future experiments. Importantly, our work suggests that for any plasmonic structure in a high permittivity dielectric, nonlocality should be taken into account.

6.3.4. Optimization and uncertainty quantification of gradient index metasurfaces

Participants: Gauthier Brière [CRHEA laboratory, Sophia Antipolis], Herbert de Gersem [TEMF institute, TU Darmstadt, Germany], Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Niklas Georg [TEMF institute, TU Darmstadt, Germany], Stéphane Lanteri, Dimitrios Loukrezis [TEMF institute, TU Darmstadt, Germany], Ulrich Römer [TEMF institute, TU Darmstadt, Germany], Nikolai Schmitt.

The design of intrinsically flat two-dimensional optical components, i.e., metasurfaces, generally requires an extensive parameter search to target the appropriate scattering properties of their constituting building blocks. Such design methodologies neglect important near-field interaction effects, playing an essential role in limiting the device performance. Optimization of transmission, phase-addressing and broadband performances of metasurfaces require new numerical tools. Additionally, uncertainties and systematic fabrication errors should be analysed. These estimations, of critical importance in the case of large production of metaoptics components, are useful to further project their deployment in industrial applications. Here, we report on a computational methodology to optimize metasurface designs. We complement this computational methodology by quantifying the impact of fabrication uncertainties on the experimentally characterized components. This analysis provides general perspectives on the overall metaoptics performances, giving an idea of the expected average behavior of a large number of devices.

NANO-D Team

6. New Results

6.1. Reconstructing molecular shapes from SAXS data

We are working on a novel method to reconstruct the three-dimensional shape of a molecule from low-resolution experimental data. The structural data we are currently focusing on is obtained through small-angle X-ray scattering (SAXS) experiments, but we plan to also consider small-angle neutron scattering (SANS) data. Our *ab initio* reconstruction method is inspired by iterative phase-retrieval algorithms that can produce an image for an object when only the amplitudes of its Fourier transform are known and the phases are unknown. In our context, the X-ray scattering amplitudes associated with a molecule are the Fourier transform of its electron density. The novelty of our approach resides in the use of spherical harmonics expansions, which will allow performing the whole reconstruction process in Fourier space—contrary to existing methods that iterate between Fourier space and real space—for an improved computational efficiency. Our method is being implemented within the software PEPSI (polynomial expansions of protein structures and interactions).

6.2. Docking of cyclic molecules

In 2018 we participated in a docking Grand Challenge 4, which was organized by the Drug Design Data Resource (D3R) group. The goal was to predict correct poses and affinities of ligands binding the beta secretase 1 (BACE) receptor. Most of the ligands were macrocyclic. The challenge answers and results were fully released in February 2019. Upon that we started analyzing our protein-ligand docking strategy and wrote a corresponding paper [5].

6.3. Convex-PL and entropy

During the 2019 we continued developing our knowledge-based scoring function for protein-ligand interactions called Convex-PL [44]. We introduced a new descriptor characterizing side-chain entropy, tried two ways of computing the solvent-accessible surface area (SASA) descriptors with either using buried SASA, or SASA of those atoms that are contributing to the protein-ligand interaction according to the scoring function design (i.e which are within the cutoff distance of an interaction potential). Using these descriptors alongwith Convex-PL score and ligand side chain entropy descriptor, we trained a ridge regression model to predict binding affinities. This modification of Convex-PL was assessed on the CASF Benchmark 2016 released in the end of 2018, and on a subset of the DUD benchmark [42]. We are currently preparing the corresponding manuscript for submission.

6.4. Orientational potential for small molecules

With Pablo Chacon and Karina Dos Santos Machado we have developed a novel statistical protein-ligand scoring function called KORP-PL. KORP-PL is based on the coarse grained backbone-only representation of protein that is very common in protein structure modeling. It is based on ideas implemented by Pablo Chacon in the preceding scoring function for protein quality assessment called KORP [49], where each amino acid residue was characterized with a 3D oriented frame. We kept this representation for protein residues and computed the distances and angles between the oriented frames and points that describe ligand atoms. Using this data, we then derived the scoring function statistically in the same way, as it was done for protein-protein interactions in KORP. We also ran an optimization procedure to compute weights for each residue-atom interaction that would minimize the difference between predicted and experimental binding constants. We have assessed KORP-PL on several benchmarks [47], [67], one of which was manually derived from the user-submitted data of the D3R Challenges 2 [35], 3 [36], and 4. On all of them it performed exceptionally in pose prediction despite being a coarse-grained scoring function. We are currently preparing the corresponding manuscript for submission.

6.5. Analysis of a deep-learning architecture for fold recognition

Deep learning has recently demonstrated outstanding capabilities in classical pattern recognition problems. It has also obtained a tremendous success in the very recent protein structure prediction tasks. This work studies recurrent structural patterns in protein structures recognized by a deep neural network. We demonstrated that neural networks can automatically learn a vast amount of chemo-structural features with only a very little amount of human supervision. For example, our architecture correctly learns atomic, amino acid, and also higher-level molecular descriptors. The network architecture and the results are available at https://team.inria.fr/nano-d/software/Ornate/.

6.6. Controlled-advancement rigid-body optimization of nanosystems

In this study, we proposed a novel optimization algorithm, with application to the refinement of molecular complexes. Particularly, we considered optimization problem as the calculation of quasi-static trajectories of rigid bodies influenced by the inverse-inertia-weighted energy gradient and introduce the concept of advancement region that guarantees displacement of a molecule strictly within a relevant region of conformational space. The advancement region helps to avoid typical energy minimization pitfalls, thus, the algorithm is suitable to work with arbitrary energy functions and arbitrary types of molecular complexes without necessary tuning of its hyper-parameters. Our method, called controlled-advancement rigid-body optimization of nanosystems (Carbon), is particularly useful for the large-scale molecular refinement, as for example, the putative binding candidates obtained with protein–protein docking pipelines. Implementation of Carbon with user-friendly interface is available in the SAMSON platform for molecular modeling at https://www.samson-connect.net. The method was published in [10].

6.7. SAXS- and SANS-assisted modeling of proteins

We collaborated on data-assisted modeling of a KRAB-domain associated protein 1. Our work sheds light on its overall organization and combins solution scattering diffraction data, integrative modeling and single-molecule experiments [3].

We also participated in a combination of coarse-grained molecular dynamics simulations with previously measured small-angle scattering data to study the conformation of three-domain protein TIA-1 in solution. More precisely, we contributed with a specifically developed version of the Pepsi-SANS code. Our results suggest a general strategy for studying the conformation of multi-domain proteins in solution that combines coarse-grained simulations with small-angle X-ray scattering data that are generally most easy to obtain [13].

6.8. Predicting protein functional motions

Large macromolecules, including proteins and their complexes, very often adopt multiple conformations. Some of them can be seen experimentally, for example with X-ray crystallography or cryo-electron microscopy. This structural heterogeneity is not occasional and is frequently linked with specific biological function. Thus, the accurate description of macromolecular conformational transitions is crucial for understanding fundamental mechanisms of life's machinery.

We report on a real-time method to predict such transitions by extrapolating from instantaneous eigen-motions, computed using the normal mode analysis, to a series of twists. We demonstrate the applicability of our approach to the prediction of a wide range of motions, including large collective opening-closing transitions and conformational changes induced by partner binding. We also highlight particularly difficult cases of very small transitions between crystal and solution structures. Our method guaranties preservation of the protein structure during the transition and allows to access conformations that are unreachable with classical normal mode analysis. We provide practical solutions to describe localized motions with a few low-frequency modes and to relax some geometrical constraints along the predicted transitions. This work opens the way to the systematic description of protein motions, whatever their degree of collectivity. Our method is available as a part of the NOn-Linear rigid Block (NOLB) package at https://team.inria.fr/nano-d/software/nolb-normal-modes/ [12].

6.9. Protein structure prediction experiments

We participated in the CAPRI Round 46, the third joint CASP-CAPRI protein assembly prediction challenge. The Round comprised a total of 20 targets including 14 homo-oligomers and 6 heterocomplexes. Eight of the homo-oligomer targets and one heterodimer comprised proteins that could be readily modeled using templates from the Protein Data Bank, often available for the full assembly. The remaining 11 targets comprised 5 homodimers, 3 heterodimers, and two higher-order assemblies. These were more difficult to model, as their prediction mainly involved “ab-initio” docking of subunit models derived from distantly related templates [7].

POEMS Project-Team

6. New Results

6.1. Complex ordered and disordered media

There is a need of a better understanding of wave phenomena in complex media. From a physical point of view, a *complex medium* is typically a material where the propagation of the waves may be *anisotropic* and *dispersive*. These properties are generally the effect of a microstructure, that can be ordered (in e.g. photonic crystals), or disordered (light in the atmosphere, seismic waves). From a mathematical point of view, one can take into account exactly this microstructure or, at sufficiently low frequency, use effective models justified by the *homogenization theory*.

6.1.1. Enriched homogenized model in presence of boundaries for time harmonic and time dependent wave equations

Participants: Clément Bénéteau, Sonia Fliss.

We study the wave equation set in a periodic half-space when the period is small compared to the wave length. The classical homogenization theory enables to derive an effective model which provides an approximation of the solution. However it is well known that these models are not accurate near the boundaries. In this work, we propose an enriched asymptotic expansion which enables to derive high order effective models at order 1 and 2. Let us mention that the model of order 2 is particularly relevant when one is interested in the long time behaviour of the solution of the time-dependent wave equation. Indeed, it is well-known that the classical homogenized model does not capture the long time dispersion of the exact solution. In several works, homogenized models of order 2 are proposed for the wave equation in infinite domains. Dealing with boundaries and proposing boundary conditions for these models of order 2 were open questions. Our approach enables to propose appropriate and accurate boundary conditions for these models. This work is the fruit of a long time collaboration with Xavier Claeys (LJLL, Sorbonne University) and a recent one with Timothée Pouchon (EPFL).

6.1.2. Interface homogenization

Participant: Jean-François Mercier.

In collaboration with Agnès Maurel from Institut Langevin and Kim Pham from the Department of Mechanics at ENSTA, we have developped interface effective models to describe acoustics and electromagnetic propagation through a scatterers array. The effective models are based on matched asymptotic expansions to account for the small thickness of the array. They consist of determined interface parameters involved in jump conditions for the fields.

1- In acoustics

• Perfect absorption using sparse arrays of Helmholtz resonators

Thanks to an effective model derived to describe a periodic arrangement of Helmholtz resonators, the influence of the spacing on the resonance has been inspected. The strength of the resonance is found enhanced when the array becomes sparser, which provides a degree of freedom to control the radiative damping of the array without affecting the losses within each resonator. It has been used to design a perfect absorbing wall.

• Scattering by arrays of open ended resonators

The previous study has been extended to cavities open at both ends. The effective model provides explicit expressions of the reflection and transmission coefficients, used to provide the relations required to produce zero reflection situation.

• Effective transmission conditions across a resonant bubbly metascreen

The extension to resonant obstacles has been considered with the study of the acoustic propagation through a thin bubbly screen. The analysis is conducted in the time domain and preserves the non linear response of the bubbles. It provides an effective model involving a jump of the normal velocity coupled to an equation of the Rayleigh-Plesset's type for the bubble radius.

2- In electromagnetism

• Perfect Brewster transmission by ultrathin perforated films

The scattering properties of an ultrathin perforated film, made of a material dielectric or perfectly conducting have been studied. Thanks to an asymptotic interface model, the Brewster incidence realizing perfect transmission is accurately described and is found to be significantly shifted from its classical value when the thickness of the film becomes subwavelength.

• Effective transmission conditions for an array of locally resonant inclusions

The previous study has been extended to resonant inclusions of the Mie type. Among the interface parameters involved in the effective model, one is frequency dependent and encapsulates the resonant behavior of the inclusions. Our effective model is validated by comparison with results of full wave calculations.

6.1.3. Wave equation in a weakly randomly perturbed periodic medium

Participants: Sonia Fliss, Laure Giovangigli.

The aim of this work, which is at its first stage, is to construct numerical approximations of the solution of the wave equation in weakly randomly perturbed periodic media in order to propose transparent boundary conditions. We start by studying the effects of rare random perturbations of the medium. The perturbation is weak in the sense that it happens rarely but when it happens the correction is of the order of the initial coefficient. More precisely, we consider the solution of the time harmonic wave equation in a one-dimensional periodic medium, in which each period have a probability η to have its coefficients modified, independently of the other periods. We derive an asymptotic expansion of the distribution of the solution u_η with respect to η and illustrate the convergence with numerical simulations. We also exhibit and implement approximated transparent boundary conditions for such a medium. We then extend the results to more general rare random perturbations. Currently, we are studying other random perturbations of periodic media such as a deformation by a random diffeomorphism with a stationary gradient.

6.1.4. Guided modes in a hexagonal periodic graph-like domain: the zigzag and the armchair cases

Participant: Sonia Fliss.

In this work, we study the wave propagation in hexagonal periodic media that are close to a graph domain. By using an asymptotic analysis, we exhibit situations where the introduction of lineic defects into the geometry of the domain leads to the appearance of guided modes and we show that the direction of the defect leads to very different properties of the guided modes. This work is done in collaboration with Bérangère Delourme (LAGA, Paris 13).

6.1.5. Stable perfectly matched layers for a class of anisotropic dispersive models

Participants: Eliane Bécache, Maryna Kachanovska.

We consider wave propagation in 2D anisotropic dispersive media in an unbounded domain described by Maxwell's equations with an antisymmetric dielectric permittivity tensor and scalar magnetic permeability. Bounding the computational domain is required to obtain the solution. In order to do so, we use the perfectly matched layer (PML) technique. However, the PMLs exhibit instabilities connected to the presence of backward propagating waves. This work is dedicated to stabilizing the PMLs for this case.

6.1.6. Frequency domain wave propagation in anisotropic metamaterials

Participants: Patrick Ciarlet, Maryna Kachanovska.

In this work we address the question of theoretical justification of problems arising in the wave propagation in hyperbolic metamaterials. Such phenomena are described by anisotropic, dispersive Maxwell equations, which, in the frequency domain, correspond to a problem that is hyperbolic for a range of frequencies. For a particular case of such materials (highly magnetized plasmas), we prove the well-posedness of the corresponding model in the free space, providing a suitable radiation condition, as well as study its regularity and demonstrate the limiting amplitude and limiting absorption principles.

6.1.7. On the analysis of perfectly matched layers for electromagnetic waves propagation in anisotropic media

Participants: Eliane Bécache, Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss, Maryna Kachanovska, Maria Kazakova.

This work consists of two parts. The first part is dedicated to the analysis of Cartesian Perfectly Matched Layers (PMLs) in the context of electromagnetic wave propagation in a 3D infinite anisotropic homogeneous medium with a diagonal dielectric tensor. Contrary to the 2D case some anisotropies lead to the existence of backward waves giving rise to instabilities of the PMLs in the time-domain and a lack of convergence in the frequency domain.

The second part examines the behaviour of the PMLs in the frequency domain in the case when in the time domain they give a rise to instabilities. This is the case e.g. for the 2D anisotropic wave equation. For this particular problem, we demonstrate that it is possible to choose the parameters of the PMLs (i.e. the configuration of the PML bounding box and the absorption parameter) to ensure the convergence of the PMLs in the frequency domain.

6.1.8. Maxwell's equations in presence of a conical tip with negative electromagnetic constants

Participants: Anne-Sophie Bonnet-Ben Dhia, Mahran Rihani.

This work is done in collaboration with Lucas Chesnel from CMAP at Ecole Polytechnique. We are interested in the analysis of time-harmonic Maxwell's equations in presence of a conical tip of a material with negative dielectric constants. When these constants belong to some critical range, the electromagnetic field exhibits strongly oscillating singularities at the tip which have infinite energy. In the 2D case of a wedge with critical electromagnetic constants, it has been proved for the equivalent scalar problems that well-posedness in the classical H^1 framework is lost. Well-posedness can be recovered (in a non standard framework) by working in weighted Sobolev spaces and adding in the space the outgoing propagating singularity. We have shown how to provide such functional framework for 3D Maxwell's equations, when only the dielectric permittivity (but not the magnetic permeability) takes a critical value

6.1.9. Essential spectrum related to an interface with a negative material

Participants: Christophe Hazard, Sandrine Paolantoni.

The studies carried out in recent years about the spectral effects of an interface between vacuum and a negative material (that is, a dispersive material whose electric permittivity and magnetic permeability become negative in some frequency range) have been continued in two directions. On the one hand, the previous theoretical studies only considered the non dissipative Drude model. We showed in particular that the interface is responsible for various resonance phenomena related to various components of an essential spectrum. We have extended these results to the so-called Lorentz model (dissipative or not). On the other hand, we have explored the numerical approximation of the spectrum of a cavity partially filled with a Drude material by considering a two-dimensional scalar problem. We have investigated the numerical simulation of the three resonance phenomena associated to the essential spectrum of the cavity.

6.1.10. Computation of plasmon resonances localized at corners using frequency-dependent complex scaling

Participants: Anne-Sophie Bonnet-Ben Dhia, Christophe Hazard, Florian Monteghetti.

A plasmonic device with a non-smooth boundary can exhibit strongly-oscillating surface waves whose phase velocities vanish as they reach the corners. This work investigates in the quasi-static limit the existence of corner resonances, which are analogous to scattering resonances in the sense that the local behavior at each corner plays the role of the behavior at infinity. Resonant contrasts are sought as eigenvalues of the transmission problem with complex scaling applied at corners.

6.1.11. Towards non-local interface models

Participant: Patrick Ciarlet.

Collaboration with Juan Pablo Borthagaray (DMEL, Universidad de la República, Salto, Uruguay). Consider the equation $\mathrm{div}(\sigma\nabla u) = f$ in Ω (plus boundary conditions), where the diffusivity is piecewise constant, and equals σ_i in Ω_i $(i = \{1, 2\})$, with $\overline{\Omega_1} \cup \overline{\Omega_2} = \overline{\Omega}$ and $\Omega_1 \cap \Omega_2 = \varnothing$. If σ_1 and σ_2 have different sign, well-posedness in $H^1(\Omega)$ may not hold. This occurs when the ratio σ_2/σ_1 belongs to the so-called *critical interval*. When the interface has a corner, we have observed that this critical interval is shrunk if one replaces the standard H^1-bilinear forms by corresponding H^s-forms ($s \in (0, 1)$). However, the expense of computing the nonlocal interactions may be prohibitive in applications. Thus, our long term goal is to confine the non-local model to a neighborhood of the interface, while keeping the standard local model in the rest of the domain. A first step in this direction consists in considering the numerical solution of the fractional Laplacian of index $s \in (1/2, 1)$ in a bounded domain Ω with homogeneous Dirichlet boundary conditions. Its solution a priori belongs to the fractional order Sobolev space $\widetilde{H}^s(\Omega)$. Under suitable assumptions on the data, its solution is also in $H^1(\Omega)$. In this case, if one uses the standard Lagrange finite element to discretize the problem, then both the exact and the computed solution belong to $H^1(\Omega)$. We show how to derive error estimates for the Lagrange finite element solutions on both quasi-uniform and graded meshes.

6.1.12. Perturbed edge finite element method for the simulation of electromagnetic waves in magnetised plasmas

Participants: Damien Chicaud, Patrick Ciarlet, Axel Modave.

Numerical simulation of electromagnetic waves in magnetised plasmas is a challenging topic. We address the finite element solution of a time-harmonic model. With the classical method, the variational formulation has a poor coercivity which leads to an ill-conditioned numerical system and numerical instabilities. We propose a perturbed formulation to improve the conditioning of the system. Promising preliminary numerical results have been obtained.

6.1.13. Resonant wave problems in plasmas

Participant: Patrick Ciarlet.

Collaboration with Martin Campos Pinto, Bruno Després and Anouk Nicolopoulos (LJLL, Sorbonne Université). The modelling of resonant waves in 2D plasma leads to the coupling of two degenerate elliptic equations. The model is set over two regions, and involves a smooth, sign-changing coefficient α. The region where $\{\alpha > 0\}$ is propagative, while the region where $\{\alpha < 0\}$ is non propagative, and elliptic. The two models are coupled through the line $\Sigma = \{\alpha = 0\}$. Generically, it is an ill-posed problem, and additional information must be introduced to get a satisfactory treatment at Σ. We define the solution by relying on the limiting absorption principle (the coefficient α is replaced by $\alpha + i0^+$) in an adapted functional setting. This approach relies on the decomposition of the solution in a regular and a singular part, which originates at Σ, and on quasi-solutions. It yields a well-posed mixed variational formulation with coupling. After the design of explicit quasi-solutions, numerical experiments can be carried out, which illustrate the nice properties of this new tool.

6.2. Towards realistic configurations : waveguides and fractals domains

To simulate realistic wave problems, devices which raise specific difficulties concerning either the modeling, the mathematical analysis or the numerical simulation. We start with propagation in *waveguides*, that is a longtime research field within our team, which has acquired an international visibility in this context. We continue with a more recent topic, propagation in *fractal* domains, motivated by a medical application (the human lung).

6.2.1. Transparent boundary conditions for periodic waveguides: analysis and extensions

Participants: Sonia Fliss, Patrick Joly.

We consider the time harmonic wave equation in perturbed periodic waveguides. We justify rigorously the construction of the transparent boundary conditions based on Dirichlet-to-Neumann map and show that the problem with these transparent boundary conditions is of Fredholm type except for a countable set of frequencies. This allows to define and compute the physical solution of the problem. This approach can be applied to deal with junctions of different periodic closed waveguides. We want now to study the extension of the method to the diffraction by locally perturbed periodic layers, surfaces or halfspaces. This work is done in collaboration with Vincent Lescarret (LSS, Centrale Supélec).

6.2.2. Invisible floating objects

Participant: Mahran Rihani.

This work is done in collaboration with Lucas Chesnel from CMAP at Ecole Polytechnique. We consider a time-harmonic water waves problem in a 2D waveguide. The geometry is symmetric with respect to an axis orthogonal to the direction of propagation of waves. Moreover, the waveguide contains two floating obstacles separated by a distance L. We study the behaviours of the scattering coefficients as L goes to ∞. From this analysis, we exhibit situations of non reflectivity or perfect invisibility.

6.2.3. A multi-trace integral equation on infinite boundaries when a global Green's function is not available

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

We are interested in time-harmonic scattering problems for configurations where the Green's function is not easily computable for the exterior domain, but different Green's functions are available in several unbounded subdomains covering the whole space. This arises typically for junctions of open waveguides. For a model problem, by using integral representations of the solution in each subdomain, we propose a formulation coupling the traces and the normal traces of the solution on infinite boundaries. The system of equations is shown to have a unique solution in the dissipative case.

6.2.4. Error analysis for transparent boundary conditions in fractal trees

Participants: Patrick Joly, Maryna Kachanovska.

This work is dedicated to an efficient resolution of the wave equation in fractal trees (with application to wave propagation in a human lung). Thanks to self-similarity, it is possible to avoid computing the solution at deeper levels of the tree by using transparent boundary conditions. The corresponding DtN operator is defined by a functional equation for its symbol. in the frequency domain. In this work, we analyse an approximate transparent condition, cf. Waves 2017, based on rational approximation of the symbol. The error and complexity analysis relies on Weyl-like estimates of eigenvalues of the weighted Laplacian and related eigenfunctions.

6.3. Direct and inverse methods for imaging and identification

Imaging and identification, when involved in a real-life context, are often based on wave propagation. This is due to the fact that a substantial part of the information contained in waves can propagate across long distances without significant attenuation. This activity is partly developed in the framework of a long-term partnership with a group of CEA-List in charge of the Non Destructive Testing (NDT) of industrial structures. The aim of NDT is to detect defects inside a structure by imposing some incident waves and measuring the scattered waves caused by the presence of such defects.

6.3.1. The complex-scaled Halfspace Matching Method

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

We are currently developing a method that we call the Half-Space Matching (HSM) method, to solve scattering problems in unbounded domains, when classical approaches are either not applicable or too expensive. This method is based on an explicit expression of the "outgoing" solution of the problem in half-spaces, by using Fourier, generalized Fourier or Floquet transforms when the background is respectively homogeneous (possibly anisotropic), stratified or periodic. The domain exterior to a bounded region enclosing the scatterers is recovered by a finite number of halfspaces (at least 3). The unknowns of the formulations are the restriction of the solution to the bounded region and the traces of the solution on the boundary of the halfspaces. The system of equations is derived by writing compatibility conditions between the different representations of the solution. Although the HSM method works in the non-dissipative case, the theoretical and the numerical analysis of the method has been done only in the dissipative case. In the present work, we propose, for the simple case of a homogeneous background, a new formulation of the method which is well-suited for the theoretical and numerical analysis of the non dissipative case. In the spirit of PMLs, the idea is to replace the system of equations on the traces by similar equations on exponentially decaying analytical extensions of the traces.

6.3.2. Implicit-explicit scheme for elastodynamic equations in plates

Participants: Sonia Fliss, Hajer Methenni.

Our objective is to provide an efficient simulation tool for the propagation of elastic waves in thin plates in the context of Guided Waves based Structural Health Monitoring. A naive discretization procedure based on a Leap-frog explicit scheme can be really costly because of the small thickness of the plate. By treating implicitly the operators corresponding to derivatives through the thickness, we show by a stability analysis that the time step is less restricted by the space discretization along the thickness. The price to pay is to solve at each iteration small independent linear systems, but this strategy offers an accurate and efficient discretization of the elastic fields in all dimensions. This method can be used to compute reference solutions and verify the validity of asymptotic models such as Reissner–Mindlin model and some extensions (since there exists no rigorous justifications for elastodynamic problems). Finally under some conditions on the mesh, our approach can be extended to plates with a smoothly varying thickness.

This work is done in collaboration with Sebastien Imperiale (Inria EPI M3DISIM) and Alexandre Imperiale (CEA-LIST).

6.3.3. Forward and inverse scattering in Kirchhoff plates

Participants: Laurent Bourgeois, Christophe Hazard.

A new activity has just started concerning forward and inverse scattering in thin plates governed by the simple Kirchhoff-Love model. The analysis is restricted to the purely bending case and the time-harmonic regime.

We have first considered a 2D strip, that is a waveguide which is unbounded in one direction and bounded in the other (transverse) direction. Two types of conditions on the boundary of the strip are addressed : 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 in the presence of a free obstacle 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. This is a joint work Lucas Chesnel, from Inria/DEFI.

We have then addressed the same kind of forward scattering problems for various impenetrable obstacles in an infinite plate. Considering four types of boundary conditions on the obstacle, well-posedness for those problems is proved with the help of a variational approach: (i) for any wave number k when the plate is clamped, simply supported or roller supported; (ii) for any k except a discrete set when the plate is free (this set is finite for convex obstacles). It is then natural to tackle the inverse problem of identifying impenetrable obstacles in a Kirchhoff-Love infinite plate from multistatic near-field data. The Linear Sampling Method is introduced in this context. We firstly prove a uniqueness result for such an inverse problem. We secondly provide the classical theoretical foundation of the Linear Sampling Method. We lastly show the feasibility of the method with the help of numerical experiments. The inverse problem is a joint work with Arnaud Recoquillay, from CEA/LIST.

6.3.4. About regularity and error estimates for the quasi-reversibility method

Participant: Laurent Bourgeois.

This work is done on collaboration with Lucas Chesnel (EPC DEFI). We are interested in the classical ill-posed Cauchy problem for the Laplace equation. One method to approximate the solution associated with compatible data consists in considering a family of regularized well-posed problems depending on a small parameter $\varepsilon > 0$. In this context, in order to prove convergence of finite elements methods, it is necessary to get regularity results of the solutions to these regularized problems which hold uniformly in ε. In the present work, we obtain these results in smooth domains and in 2D polygonal geometries. In the presence of corners, due to the particular structure of the regularized problems, classical techniques *à la* Grisvard do not work and instead, we apply the Kondratiev approach. We describe the procedure in detail to keep track of the dependence in ε in all the estimates. The main originality of this study lies in the fact that the limit problem is ill-posed in any framework.

6.3.5. Analysis of topological derivative as a means for qualitative identification

Participant: Marc Bonnet.

This work is done on collaboration with Fioralba Cakoni, Rutgers University, USA. The concept of topological derivative (TD) has proved effective as a qualitative inversion tool for a wave-based identification of finite-sized objects. Although for the most part, this approach remains based on a heuristic interpretation of the TD, a first attempt toward its mathematical justification was done in Bellis et al. (*Inverse Problems***29**:075012, 2013) for the case of isotropic media with far field data and inhomogeneous refraction index. This work extends the analysis there to the case of anisotropic scatterers and background with near field data. TD-based imaging functional is analyzed using a suitable factorization of the near fields. Our results include justification of sign heuristics for the TD in the isotropic case with jump in the main operator and for some cases of anisotropic media, as well as verifying its decaying property in the isotropic case with near field spherical measurements configuration situated far enough from the probing region.

6.3.6. Asymptotic model for elastodynamic scattering by a small surface-breaking defect

Participant: Marc Bonnet.

This work is done in collaboration with Marc Deschamps and Eric Ducasse, I2M, Bordeaux.

We establish a leading-order asymptotic model for the scattering of elastodynamic fields by small surface-breaking defects in elastic solids. The asymptotic form of the representation formula of the scattered field is written in terms of the elastodynamic Green's tensor, which is in fact available in semi-analytical form for some geometrical configurations that are of practical interest in ultrasonic NDT configurations. Preliminary numerical examples have been performed on cylindrical elastic pipes with small indentations on the outer surface.

6.3.7. Shape optimization of stokesian peristaltic pumps using boundary integral methods

Participant: Marc Bonnet.

This work is done in collaboration with with Ruowen Liu and Shravan Veerapaneni, University of Michigan, USA.

This work develops a new boundary integral approach for finding optimal shapes of peristaltic pumps that transport a viscous fluid. Formulas for computing the shape derivatives of the standard cost functionals and constraints, expressed in boundary-only form, are derived. They involve evaluating physical variables (traction, pressure, etc.) on the boundary only. By employing these formulas in conjunction with a boundary integral approach for solving forward and adjoint problems, we completely avoid the issue of volume remeshing when updating the pump shape as the optimization proceeds. This leads to significant cost savings and we demonstrate the performance on several numerical examples.

6.4. Accelerated numerical solvers for large-scale wave problems

Fast solution procedures are of critical importance for industrial applications such as non-destructive testing, electromagnetic compatibility testing and seismic risk assessment. In these examples, the wavelength is very small in comparison to the characteristic length of the problems, which leads to extremely expensive numerical procedures if standard methods are used. To address the fast numerical solution of large-scale waves problems, we work at the same time on numerical methods, algorithmic issues and implementation strategies to speed up solvers.

6.4.1. Non-overlapping Domain Decomposition Method (DDM) using non-local transmission operators for wave propagation problems.

Participants: Patrick Joly, Emile Parolin.

The research in this direction was mainly concerned by the extension to the electromagnetic setting of the linear convergence theory of non-overlapping DDM that relies on non-local transmission operators. The principal task was to propose, analyse and implement some candidate non-local operators satisfying the assumptions of the theory. There were two main propositions:

- Integral operator for the electromagnetic setting: the operator is available in closed form and its structure lead naturally to a localizable form via truncation of the kernel to limit the effective computational cost while retaining its good properties. The construction of such an operator turned out to be somewhat difficult due to the particular functional setting of Maxwell's equations.
- DtN based non-local operator: the operator is computed by solving auxiliary coercive problems in the vicinity of the transmission interface. The computational cost remains moderate as the implementation no longer involve dense matrix blocks from the integral operators but rather lead to augmented sparse linear systems. Initially developed for the electromagnetic setting, the approach is appealing as it provided a unified formalism that can be applied both to Helmholtz and Maxwell equations and proved to be efficient in numerical experiments.

Another important research direction is created by the technical and theoretical difficulty posed by junction points, which are points where three or more sub-domains abut. Xavier Claeys recently proposed a method to deal with this specific issue, based on the multi-trace formalism, which led to a joint collaboration on the subject. The main idea is to perform a global exchange operation, on the whole skeleton, rather than a local point-to-point exchange. The preliminary numerical results recently obtained are promising.

6.4.2. An efficient domain decomposition method with cross-point treatment for Helmholtz problems

Participant: Axel Modave.

This is a collaboration with X. Antoine (IECL, Nancy), A. Royer (ULiège) and C. Geuzaine (ULiège). The parallel finite-element solution of large-scale time-harmonic scattering problems is addressed with a non-overlapping domain decomposition method (DDM). It is well known that the efficiency of this method strongly depends on the transmission condition enforced on the interfaces between the subdomains. Local conditions based on high-order absorbing boundary conditions (HABCs) are well suited for configurations without cross points *(where more than two subdomains meet)*. In this work, we extend this approach to efficiently deal with cross points. Two-dimensional finite-element results are presented.

6.4.3. Modelling the fluid-structure coupling caused by a far-field underwater explosion using a convolution quadrature based fast boundary element method.

Participants: Marc Bonnet, Stéphanie Chaillat, Damien Mavaleix-Marchessoux.

This study is done in collaboration with Bruno Leblé (Naval Group). It aims at developing computational strategies for modelling the impact of a far-field underwater explosion shock wave on a structure, in deep water. An iterative fluid-structure coupling is developed to solve the problem. Two complementary methods are used: the Finite Element Method (FEM), that offers a wide range of tools to compute the structure response; and the Boundary Element Method (BEM), more suitable to deal with large surrounding fluid domains. We concentrate on developing (i) a fast transient BEM procedure and (ii) a transient FEM-BEM coupling algorithm. The fast transient BEM is based on a fast multipole-accelerated Laplace-domain BEM (implemented in the in-house code COFFEE), extended to the time domain by the Convolution Quadrature Method (CQM). In particular, using empirical approximations for the solution of integral problems involving large (complex) frequencies has been found to yield satisfactorily accurate solutions while saving significant amounts of computational work. The transient BEM-FEM coupling (under progress) will be based on a block-SOR iterative approach, for which a preliminary investigation shows the existence of relaxation parameters that ensure convergence.

6.4.4. Asymptotic based methods for very high frequency problems.

Participant: Eric Lunéville.

This research is developed in collaboration with Marc Lenoir and Daniel Bouche (CEA).

It has recently been realized that the combination of integral and asymptotic methods was a remarkable and necessary tool to solve scattering problems, in the case where the frequency is high and the geometry must be finely taken into account.

In order to implement the high-frequency approximations that we are developing as part of these hybrid HF/BF methods, we have introduced new geometric tools into the XLiFE++ library, in particular splines and B-Splines approximations as well as parameterizations to access quantities such as curvature, curvilinear abscissa, etc. We have also started to interface the OpenCascad library to the XLiFE++ library, which will eventually allow us to manage more complex geometric situations (cylinder and sphere intersection for example). In parallel, we have completed the implementation of 2D HF approximations in the shadow-light transition zone based on the Fock function. Diffraction by a 2D corner is in progress.

RAPSODI Project-Team

7. New Results

7.1. Modeling and numerical simulation of complex fluids

In [38], N. Peton, C. Cancès *et al.* propose a new water flow driven forward stratigraphic model. Stratigraphy is a discipline of physics that aims at predicting the geological composition of the subsoil. The model enjoys 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.

In [14], A. Ait Hammou Oulhaj and D. Maltese adapt the (positive) nonlinear Control Volume Finite Element scheme of [83] to the simulation of seawater intrusion in the subsoil nearby coastal regions. The proposed scheme is convergent even if the porous medium is anisotropic.

In [25], [41], C. Cancès *et al.* study an original model of degenerate Cahn–Hilliard type. Similarly to the classical degenerate Cahn–Hilliard model, the model can be interpreted as the gradient flow of a Ginzburg–Landau type energy, but the geometry considered here allows for more flexibility and the system thus dissipates faster than the usual degenerate Cahn–Hilliard system. Numerical evidences of this fact are given. Then, the existence of a solution to the model is established thanks to the convergence of a minimizing movement scheme.

In [19], 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 [80]. 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, I. 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 [97], [100].

In [22], C. Calgaro, C. Colin, 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.* [103], [104].

In [21], C. Calgaro, C. Colin, and E. Creusé derive 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 [74], [101], [69], as well as in the natural convection of a flow in a cavity [108], [105], [101], [69].

In [20], C. Calgaro, C. Colin, and E. Creusé propose a combined Finite Volume-Finite Element scheme for the solution of a specific low-Mach model expressed in the velocity, pressure and temperature variables. The dynamic viscosity of the fluid is given by an explicit function of the temperature, leading to the presence of a so-called Joule term in the mass conservation equation. First, they prove a discrete maximum principle for the temperature. Second, the numerical fluxes defined for the Finite Volume computation of the temperature are efficiently derived from the discrete Finite Element velocity field obtained by the solution of the momentum equation. Several numerical tests are presented to illustrate the theoretical results and to underline the efficiency of the scheme in terms of convergence rates.

In [46], C. Calgaro and E. Creusé introduce a Finite Volume method to approximate the solution of a convection-diffusion equation involving a Joule term. They propose a way to discretize this so-called "Joule effect" term in a consistent manner with respect to the nonlinear diffusion one, in order to ensure some maximum principle properties on the solution. They investigate the numerical behavior of the scheme on two original benchmarks.

7.2. Numerical simulation in low-frequency electromagnetism

In [32], [31], E. Creusé *et al.* 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. A more theoretical contribution is also developed to prove the equivalence of some usual discrete gauge conditions. Once again, their numerical behaviors are compared on some characteristic benchmarks.

In [58], F. Chave, S. Lemaire *et al.* introduce a three-dimensional Hybrid High-Order (HHO) method for magnetostatic problems. The proposed method is easy to implement, supports general polyhedral meshes, and allows for arbitrary orders of approximation.

7.3. Structure-preserving numerical methods

In [54], C. Cancès *et al.* 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.

In [55], C. Chainais-Hillairet and M. Herda apply an iterative energy method à la de Giorgi in order to establish L^∞ bounds for numerical solutions of noncoercive convection-diffusion equations with mixed Dirichlet-Neumann boundary conditions.

In [23], C. Cancès, C. Chainais-Hillairet *et al.* study a finite volume scheme for a degenerate cross-diffusion system describing the ion transport through biological membranes. 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 finite volume scheme is based on two-point flux approximations with "double" upwind mobilities. The existence of solutions to the fully discrete scheme is proven. When the particles are not distinguishable and the dynamics is driven by cross-diffusion only, it is shown that the scheme preserves the structure of the equations like nonnegativity, upper bounds, and entropy dissipation.

In [51], C. Cancès and B. Gaudeul propose a two-point flux approximation finite volume scheme for the approximation of the solutions to an entropy dissipative cross-diffusion system. The scheme is shown to preserve several key properties of the continuous system, among which positivity and decay of the entropy. Numerical experiments illustrate the behavior of the scheme.

In [48], C. Cancès, C. Chainais-Hillairet, B. Gaudeul *et al.* consider an unipolar degenerate drift-diffusion system arising in the modeling of organic semiconductors. They design four different finite volume schemes based on four different formulations of the fluxes. They provide a stability analysis and existence results for the four schemes; the convergence is established for two of them.

In [24], C. Cancès *et al.* compare energy-stable finite volume schemes for multiphase flows in porous media with schemes based on the Wasserstein gradient flow structure of the equations, that has recently been highlighted in [3]. The model is approximated by means of the minimizing movement (or JKO) scheme, that C. Cancès *et al.* solve thanks to the ALG2-JKO scheme proposed in [76].

In [50], C. Cancès *et al.* propose a variational finite volume scheme for the computation of Wasserstein gradient flows. The discrete solution is the minimizer of a discrete action, keeping track at the discrete level of the optimal character of the gradient flow. The spatial discretization relies on upstream mobility fluxes, while an implicit linearization of the Wasserstein distance is used in order to reduce the computational cost by avoiding an inner time-stepping as in the related contributions of the literature.

In [61], T. Rey *et al.* present a new finite volume method for computing numerical approximations of a system of nonlocal transport equations modeling interacting species. In this work, the nonlocal continuity equations are treated as conservative transport equations with a nonlocal, nonlinear, rough velocity field. Some properties of the method are analyzed, and numerical simulations are performed.

In [15], 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 [78] 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.

7.4. Cost reduction for numerical methods

In [36], S. Lemaire builds a bridge between the Hybrid High-Order [93] and Virtual Element [75] 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. Here, 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 as it sheds new light on the *a priori* analysis of Virtual Element methods, and on the differences between the conforming and nonconforming cases.

In [30], [40], S. Lemaire *et al.* design and analyze (in the periodic setting) arbitrary-order nonconforming multiscale methods for highly oscillatory elliptic problems, which are applicable on coarse grids that may feature general polytopal cells. The construction of these methods is based on the Hybrid High-Order framework [93]. 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 [52], C. Cancès and D. Maltese propose a reduced model for the migration of hydrocarbons in heterogeneous porous media. Their model keeps track of the time variable. This allows to compute steady-states that cannot be reached by the commonly used ray-tracing and invasion-percolation algorithms. An efficient finite volume scheme allowing for very large time steps is then proposed.

In [57], F. Chave proposes a new definition of the normal fracture diffusion-dispersion coefficient for a reduced model of passive transport in fractured porous media, and numerically studies the impact on the discrete solution on a few test-cases.

In [37], 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. The method is illustrated with numerical results in one and two space dimensions.

In [60], I. Lacroix-Violet *et al.* introduce a new class of numerical methods for the time integration of evolution equations set as Cauchy problems of ODEs or PDEs. The systematic design of these methods mixes the Runge–Kutta collocation formalism with collocation techniques, in such a way that the methods are linearly implicit and have high order. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods are expected to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so.

7.5. Asymptotic analysis

In [18], C. Cancès *et al.* 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 particles follow a degenerate dynamics, in the sense that the jump rates can vanish for certain configurations, and there exist blocked configurations that cannot evolve. Our approach, which is based on the relative entropy method, is tailored to deal with vanishing initial densities.

In [13], A. Ait Hammou Oulhaj, C. Cancès, C. Chainais-Hillairet *et al.* study the large-time behavior of the solutions to a two-phase extension of the porous media equation, which models the seawater intrusion problem. Their goal is to identify the self-similar solutions that correspond to steady-states of a rescaled version of the problem. They fully characterize the unique steady-states that are identified as minimizers of a convex energy and shown to be radially symmetric. Moreover, they prove the convergence of the solution to the time-dependent model towards the unique stationary state as time goes to infinity. They also provide numerical illustrations of the stationary states and exhibit numerical convergence rates.

In [16], C. Chainais-Hillairet *et al.* propose a new proof of existence of a solution to the scheme introduced in [1] for drift-diffusion systems, 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 [1].

In [26], C. Chainais-Hillairet and M. Herda study the large-time behavior of the 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 [49], C. Cancès, C. Chainais-Hillairet, M. Herda *et al.* analyze the large-time behavior of a family of nonlinear finite volume schemes for anisotropic convection-diffusion equations set in a bounded bidimensional domain and endowed with either Dirichlet and/or no-flux boundary conditions. They show that the solutions to the two-point flux approximation (TPFA) and discrete duality finite volume (DDFV) schemes under consideration converge exponentially fast toward their steady-state. The analysis relies on discrete entropy estimates and discrete functional inequalities. As a by-product of their analysis, they establish new discrete Poincaré–Wirtinger, Beckner and logarithmic Sobolev inequalities. Their theoretical results are illustrated by numerical simulations.

In [56], C. Chainais-Hillairet *et al.* introduce a nonlinear DDFV scheme for an anisotropic linear convection-diffusion equation with mixed boundary conditions and establish the exponential decay of the scheme towards its steady-state.

In [39], A. Zurek studies the large-time regime of the moving interface appearing in a concrete carbonation model. He proves that the approximate free boundary, given by an implicit-in-time Finite Volume scheme, propagates in time following a $\sqrt{t}$-law. This result is illustrated by numerical experiments.

In [17], 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 in [95] 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 [44], M. Herda *et al.* are interested in the large-time behavior of linear kinetic equations with heavy-tailed local equilibria. Their main contribution concerns the kinetic Lévy–Fokker–Planck equation, for which they adapt hypocoercivity techniques in order to show that solutions converge exponentially fast to the global equilibrium. Compared to the classical kinetic Fokker–Planck equation, the issues here concern the lack of symmetry of the non-local Lévy–Fokker–Planck operator and the understanding of its regularization properties. As a complementary related result, they also treat the case of the heavy-tailed BGK equation.

In [35], 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.

In [45], T. Rey *et al.* propose a new mathematical model intended to describe dynamically the evolution of knowledge in structured societies of interacting individuals. This process, termed cumulative culture, has been extensively studied by evolutionary anthropologists, both theoretically and experimentally. Some of the mathematical properties of the new model are analyzed, and exponential convergence towards a global equilibrium is shown for a simplified model. A numerical method is finally proposed to simulate the complete model.

In [43], following the ideas of V. V. Zhikov and A. L. Pyatnitskii, and more precisely the stochastic two-scale convergence, B. Merlet *et al.* establish a homogenization theorem in a stochastic setting for two nonlinear equations: the equation of harmonic maps into the sphere and the Landau–Lifshitz equation. Homogenization results for nonlinear problems are known to be difficult. In this particular case the equations have strong nonlinear features, in particular, in general their solutions are not unique. Here the authors take advantage of the different equivalent definitions of weak solutions to the nonlinear problem to apply typical linear homogenization recipes.

7.6. Applied calculus of variations

In [34], 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 [112]). 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 [27], B. Merlet *et al.* consider the branched transportation problem in 2D associated with a cost per unit length of the form $1 + \beta\theta$ where θ denotes the amount of transported mass and $\beta > 0$ is a fixed parameter (notice that the limit case $\beta = 0$ corresponds to the classical Steiner problem). Motivated by the numerical approximation of this problem, they introduce a family of functionals ($\{\mathcal{F}_\varepsilon\}_{\varepsilon>0}$) which approximate the above branched transport energy. They justify rigorously the approximation by establishing the equicoercivity and the Γ-convergence of $\{\mathcal{F}_\varepsilon\}$ as $\varepsilon \downarrow 0$. The functionals are modeled on the Ambrosio–Tortorelli functional and are easy to optimize in practice. Numerical evidences of the efficiency of the method are presented.

In [28], 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 [29].

In [29], B. Merlet *et al.* consider a generalization of branched transportation 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 transportation problem is established 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 [33], [62], B. Merlet *et al.* study a family of functionals penalizing oblique oscillations. These functionals naturally appear in some variational problems related to pattern formation and are somewhat reminiscent of those introduced by Bourgain, Brezis and Mironescu to characterize Sobolev functions. More precisely, for a function u defined on a tensor product $\Omega_1 \times \Omega_2$, the family of functionals $\{E_\varepsilon(u)\}_{\varepsilon>0}$ that we consider vanishes if u is of the form $u(x_1)$ or $u(x_2)$. We prove the converse property and related quantitative results. In particular, we describe the fine properties of functions with $\sup_\varepsilon E_\varepsilon(u) < \infty$ by showing that roughly, such u is piecewise of the form $u(x_1)$ or $u(x_2)$ on domains separated by lines where the energy concentrates. It turns out that this problem naturally leads to the study of various differential inclusions and has connections with branched transportation models.

7.7. Approximation theory

In [59], M. Herda *et al.* propose an iterative algorithm for the numerical computation of sums of squares of polynomials approximating given data at prescribed interpolation points. The method is based on the definition of a convex functional G arising from the dualization of a quadratic regression over the Cholesky factors of the sum of squares decomposition. In order to justify the construction, the domain of G, the boundary of the domain and the behavior at infinity are analyzed in details. When the data interpolate a positive univariate polynomial, we show that in the context of the Lukacs sum of squares representation, G is coercive and strictly convex which yields a unique critical point and a corresponding decomposition in sum of squares. For multivariate polynomials which admit a decomposition in sum of squares and up to a small perturbation of size ε, G^ε is always coercive and so its minimum yields an approximate decomposition in sum of squares. Various unconstrained descent algorithms are proposed to minimize G. Numerical examples are provided, for univariate and bivariate polynomials.

In [47], M. Herda *et al.* investigate the numerical approximation of bounded functions by polynomials satisfying the same bounds. The contribution makes use of the recent algebraic characterization found in [91] and [92] where an interpretation of monovariate polynomials with two bounds is provided in terms of a quaternion algebra and the Euler four-squares formulas. Thanks to this structure, the authors generate a new nonlinear projection algorithm onto the set of polynomials with two bounds. The numerical analysis of the method provides theoretical error estimates showing stability and continuity of the projection. Some numerical tests illustrate this novel algorithm for constrained polynomial approximation.

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 [12] we propose a variational model for joint image reconstruction and motion estimation applicable to spatiotemporal imaging. This model consists of two parts, one that conducts image reconstruction in a static setting and another that estimates the motion by solving a sequence of coupled indirect image registration problems, each formulated within the large deformation diffeomorphic metric mapping framework. The proposed model is compared against alternative approaches (optical flow based model and diffeomorphic motion models). Next, we derive efficient algorithms for a time-discretized setting and show that the optimal solution of the time-discretized formulation is consistent with that of the time-continuous one. The complexity of the algorithm is characterized and we conclude by giving some numerical examples in 2D space + time tomography with very sparse and/or highly noisy data.
- The article [16] presents a method to incorporate a deformation prior in image reconstruction via the formalism of deformation modules. The framework of deformation modules allows to build diffeomorphic deformations that satisfy a given structure. The idea is to register a template image against the indirectly observed data via a modular deformation, incorporating this way the deformation prior in the reconstruction method. We show that this is a well-defined regularization method (proving existence, stability and convergence) and present numerical examples of reconstruction from 2-D tomographic simulations and partially-observed images.
- The article [28] adapts the framework of metamorphosis to the resolution of inverse problems with shape prior. The metamorphosis framework allows to transform an image via a balance between geometrical deformations and changes in intensities (that can for instance correspond to the appearance of a new structure). The idea developed here is to reconstruct an image from noisy and indirect observations by registering, via metamorphosis, a template to the observed data. Unlike a registration with only geometrical changes, this framework gives good results when intensities of the template are poorly chosen. We show that this method is a well-defined regularization method (proving existence, stability and convergence) and present several numerical examples.
- In [8] 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 [33] we show that, for a sub-Laplacian Δ on a 3-dimensional manifold M, no point interaction centered at a point $q_0 \in M$ exists.
- In [39] we consider a one-parameter family of Grushin-type singularities on surfaces, and discuss the possible diffusions that extend Brownian motion to the singularity. This gives a quick proof and clear intuition for the fact that heat can only cross the singularity for an intermediate range of the parameter. When crossing is possible and the singularity consists of one point, we give a complete description of these diffusions, and we describe a “best" extension, which respects the isometry group of the surface and also realizes the unique symmetric one-point extension of the Brownian motion, in the sense of Chen-Fukushima. This extension, however, does not correspond to the bridging extension, which was introduced by Boscain-Prandi, when they previously considered self-adjoint extensions of the Laplace-Beltrami operator on the Riemannian part for these surfaces. We clarify that several of the extensions they considered induce diffusions that are carried by the Marin compactification at the singularity, which is much larger than the (one-point) metric

completion. In the case when the singularity is more than one-point, a complete classification of diffusions extending Brownian motion would be unwieldy. Nonetheless, we again describe a “best" extension which respects the isometry group, and in this case, this diffusion corresponds to the bridging extension. A prominent role is played by Bessel processes (of every real dimension) and the classical theory of one-dimensional diffusions and their boundary conditions.

- In [50] 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 monograph [30] and the PhD thesis of Mathieu Kohli [3].

6.2. Quantum control: new results

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

- In [29], we discuss the compatibility between the rotating-wave and the adiabatic approximations for controlled quantum systems. Although the paper focuses on applications to two-level quantum systems, the main results apply in higher dimension. Under some suitable hypotheses on the time scales, the two approximations can be combined. As a natural consequence of this, it is possible to design control laws achieving transitions of states between two energy levels of the Hamiltonian that are robust with respect to inhomogeneities of the amplitude of the control input.
- In [34] we study one-parametric perturbations of finite dimensional real Hamiltonians depending on two controls, and we show that generically in the space of Hamiltonians, conical intersections of eigenvalues can degenerate into semi-conical intersections of eigenvalues. Then, through the use of normal forms, we study the problem of ensemble controllability between the eigenstates of a generic Hamiltonian.
- In [35] we discuss which controllability properties of classical Hamiltonian systems are preserved after quantization. We discuss some necessary and some sufficient conditions for small-time controllability of classical systems and quantum systems using the WKB method. In particular, we investigate the conjecture that if the classical system is not small-time controllable, then the corresponding quantum system is not small-time controllable either.
- In [40] we study the controllability problem for a symmetric-top molecule, both for its classical and quantum rotational dynamics. As controlled fields we consider three orthogonally polarized electric fields which interact with the electric dipole of the molecule. We characterize the controllability in terms of the dipole position: when it lies along the symmetry axis of the molecule nor the classical neither the quantum dynamics are controllable, due to the presence of a conserved quantity, the third component of the total angular momentum; when it lies in the orthogonal plane to the symmetry axis, a quantum symmetry arises, due to the superposition of symmetric states, which as no classical counterpart. If the dipole is neither along the symmetry axis nor orthogonal to it, controllability for the classical dynamics and approximate controllability for the quantum dynamics is proved to hold.

We would also like to mention the defense of the PhD thesis of Nicolas Augier (not yet on TEL) on the subject.

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 an open channel, a hydraulic jump is an abrupt transition between a torrential (super-critical) flow and a fluvial (subcritical) flow. In [9] hydraulic jumps are represented by discontinuous shock solutions of hyperbolic Saint-Venant equations. Using a Lyapunov approach, we prove that we can stabilize the state of the system in H^2-norm as well as the hydraulic jump location, with simple feedback boundary controls and an arbitrary decay rate, by appropriately choosing the gains of the feedback boundary controls.

- In [10], 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.
- We develop in [19] a method ensuring robustness properties to bang-bang strategies , for general nonlinear control systems. Our main idea is to add bang arcs in the form of needle-like variations of the control. With such bang-bang controls having additional degrees of freedom, steering the control system to some given target amounts to solving an overdetermined nonlinear shooting problem, what we do by developing a least-square approach. In turn, we design a criterion to measure the quality of robustness of the bang-bang strategy, based on the singular values of the end-point mapping, and which we optimize. Our approach thus shows that redundancy implies robustness, and we show how to achieve some compromises in practice, by applying it to the attitude control of a 3d rigid body.
- Partial stability characterizes dynamical systems for which only a part of the state variables exhibits a stable behavior. In his book on partial stability, Vorotnikov proposed a sufficient condition to establish this property through a Lyapunov-like function whose total derivative is upper-bounded by a negative definite function involving only the sub-state of interest. In [20], we show with a simple two-dimensional system that this statement is wrong in general. More precisely, we show that the convergence rate of the relevant state variables may not be uniform in the initial state. We also discuss the impact of this lack of uniformity on the connected issue of robustness with respect to exogenous disturbances.
- The paper [21] 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).
- The goal of [23] 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. An 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.
- Given a linear control system in a Hilbert space with a bounded control operator, we establish in [26] 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 [37] we propose an extension of the theory of control sets to the case of inputs satisfying a dwell-time constraint. Although the class of such inputs is not closed under concatenation, we propose a

suitably modified definition of control sets that allows to recover some important properties known in the concatenable case. In particular we apply the control set construction to dwell-time linear switched systems, characterizing their maximal Lyapunov exponent looking only at trajectories whose angular component is periodic. We also use such a construction to characterize supports of invariant measures for random switched systems with dwell-time constraints.

- In [41] we study asymptotic stability of continuous-time systems with mode-dependent guaranteed dwell time. These systems are reformulated as special cases of a general class of mixed (discrete-continuous) linear switching systems on graphs, in which some modes correspond to discrete actions and some others correspond to continuous-time evolutions. Each discrete action has its own positive weight which accounts for its time-duration. We develop a theory of stability for the mixed systems; in particular, we prove the existence of an invariant Lyapunov norm for mixed systems on graphs and study its structure in various cases, including discrete-time systems for which discrete actions have inhomogeneous time durations. This allows us to adapt recent methods for the joint spectral radius computation (Gripenberg's algorithm and the Invariant Polytope Algorithm) to compute the Lyapunov exponent of mixed systems on graphs.
- Given a discrete-time linear switched system associated with a finite set of matrices, we consider the measures of its asymptotic behavior given by, on the one hand, its deterministic joint spectral radius and, on the other hand, its probabilistic joint spectral radius for Markov random switching signals with given transition matrix and corresponding invariant probability. In [42], we investigate the cases of equality between the two measures.
- In [45] 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 [46] 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.
- In [47] 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.
- In [48], we address the problem of the exponential stability of density-velocity systems with boundary conditions. Density-velocity systems are omnipresent in physics as they encompass all systems that consist in a flux conservation and a momentum equation. In this paper we show that any such system can be stabilized exponentially quickly in the H^2 norm using simple local feedbacks, provided a condition on the source term which holds for most physical systems, even when it is not

dissipative. Besides, the feedback laws obtained only depends on the target values at the boundaries, which implies that they do not depend on the expression of the source term or the force applied on the system and makes them very easy to implement in practice and robust to model errors. For instance, for a river modeled by Saint-Venant equations this means that the feedback laws do not require any information on the friction model, the slope or the shape of the channel considered. This feat is obtained by showing the existence of a basic H^2 Lyapunov functions and we apply it to numerous systems: the general Saint-Venant equations, the isentropic Euler equations, the motion of water in rigid-pipe, the osmosis phenomenon, etc.

- The general context of [56] is the feedback control of an infinite-dimensional system so that the closed-loop system satisfies a fading-memory property and achieves the setpoint tracking of a given reference signal. More specifically , this paper is concerned with the Proportional Integral (PI) regulation control of the left Neumann trace of a one-dimensional reaction-diffusion equation with a delayed right Dirichlet boundary control. In this setting, the studied reaction-diffusion equation might be either open-loop stable or unstable. The proposed control strategy goes as follows. First, a finite-dimensional truncated model that captures the unstable dynamics of the original infinite-dimensional system is obtained via spectral decomposition. The truncated model is then augmented by an integral component on the tracking error of the left Neumann trace. After resorting to the Artstein transformation to handle the control input delay, the PI controller is designed by pole shifting. Stability of the resulting closed-loop infinite-dimensional system, consisting of the original reaction-diffusion equation with the PI controller, is then established thanks to an adequate Lyapunov function. In the case of a time-varying reference input and a time-varying distributed disturbance, our stability result takes the form of an exponential Input-to-State Stability (ISS) estimate with fading memory. Finally, another exponential ISS estimate with fading memory is established for the tracking performance of the reference signal by the system output. In particular, these results assess the setpoint regulation of the left Neumann trace in the presence of distributed perturbations that converge to a steady-state value and with a time-derivative that converges to zero. Numerical simulations are carried out to illustrate the efficiency of our control strategy.
- There exist many ways to stabilize an infinite-dimensional linear autonomous control systems when it is possible. Anyway, finding an exponentially stabilizing feedback control that is as simple as possible may be a challenge. The Riccati theory provides a nice feedback control but may be computationally demanding when considering a discretization scheme. Proper Orthogonal Decomposition (POD) offers a popular way to reduce large-dimensional systems. In [59], we establish that, under appropriate spectral assumptions, an exponentially stabilizing feedback Riccati control designed from a POD finite-dimensional approximation of the system stabilizes as well the infinite-dimensional control system.
- In [60] we consider a 1-D linear transport equation on the interval $(0, L)$, with an internal scalar control. We prove that if the system is controllable in a periodic Sobolev space of order greater than 1, then the system can be stabilized in finite time, and we give an explicit feedback law.
- In [61] 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.

6.4. Controllability: new results

Let us list here our new results on controllability beyond the quantum control framework.

- In [13], we study approximate and exact controllability of linear difference equations using as a basic tool a representation formula for its solution in terms of the initial condition, the control, and some suitable matrix coefficients. When the delays are commensurable, approximate and exact controllability are equivalent and can be characterized by a Kalman criterion. The paper focuses on providing characterizations of approximate and exact controllability without the commensurability assumption. In the case of two-dimensional systems with two delays, we obtain an explicit characterization of approximate and exact controllability in terms of the parameters of the problem. In the general setting, we prove that approximate controllability from zero to constant states is equivalent to approximate controllability in L^2. The corresponding result for exact controllability is true at least for two-dimensional systems with two delays.

- In [14] we consider the 2D incompressible Navier-Stokes equation in a rectangle with the usual no-slip boundary condition prescribed on the upper and lower boundaries. We prove that for any positive time, for any finite energy initial data, there exist controls on the left and right boundaries and a distributed force, which can be chosen arbitrarily small in any Sobolev norm in space, such that the corresponding solution is at rest at the given final time. Our work improves earlier results where the distributed force is small only in a negative Sobolev space. It is a further step towards an answer to Jacques-Louis Lions' question about the small-time global exact boundary controllability of the Navier-Stokes equation with the no-slip boundary condition, for which no distributed force is allowed. Our analysis relies on the well-prepared dissipation method already used for Burgers and for Navier-Stokes in the case of the Navier slip-with-friction boundary condition. In order to handle the larger boundary layers associated with the no-slip boundary condition, we perform a preliminary regularization into analytic functions with arbitrarily large analytic radius and prove a long-time nonlinear Cauchy-Kovalevskaya estimate relying only on horizontal analyticity.
- We consider the wave equation on a closed Riemannian manifold. We observe the restriction of the solutions to a measurable subset ω along a time interval $[0, T]$ with $T > 0$. It is well known that, if ω is open and if the pair (ω, T) satisfies the Geometric Control Condition then an observability inequality is satisfied, comparing the total energy of solutions to their energy localized in $\omega \times (0, T)$. The observability constant $C_T(\omega)$ is then defined as the infimum over the set of all nontrivial solutions of the wave equation of the ratio of localized energy of solutions over their total energy. In [17], we provide estimates of the observability constant based on a low/high frequency splitting procedure allowing us to derive general geometric conditions guaranteeing that the wave equation is observable on a measurable subset ω. We also establish that, as $T \to +\infty$, the ratio $C_T(\omega)/T$ converges to the minimum of two quantities: the first one is of a spectral nature and involves the Laplacian eigenfunctions, the second one is of a geometric nature and involves the average time spent in ω by Riemannian geodesics.
- In [22] 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.
- The paper [27] deals with the controllability problem of a linearized Korteweg-de Vries equation on bounded interval. The system has a homogeneous Dirichlet boundary condition and a homogeneous Neumann boundary condition at the right end-points of the interval, a non homogeneous Dirichlet boundary condition at the left end-point which is the control. We prove the null controllability by using a backstepping approach, a method usually used to handle stabilization problems.
- The paper [44] is devoted to the controllability of a general linear hyperbolic system in one space dimension using boundary controls on one side. Under precise and generic assumptions on the boundary conditions on the other side, we previously established the optimal time for the null and

the exact controllability for this system for a generic source term. In this work, we prove the null-controllability for any time greater than the optimal time and for any source term. Similar results for the exact controllability are also discussed.

- Given any measurable subset ω of a closed Riemannian manifold and given any $T > 0$, we study in [49] the smallest average time over $[0, T]$ spent by all geodesic rays in ω. This quantity appears naturally when studying observability properties for the wave equation on M, with ω as an observation subset.
- Our goal is to study controllability and observability properties of the 1D heat equation with internal control (or observation) set an interval of size $\epsilon \to 0$. For any ϵ fixed, the heat equation is controllable in any time $T > 0$. It is known that depending on arithmetic properties of the center of the interval, there may exist a minimal time of pointwise control of the heat equation. We relate these two phenomena in [54].
- Our goal in [55] is to relate the observation (or control) of the wave equation on observation domains which evolve in time with some dynamical properties of the geodesic flow. In comparison to the case of static domains of observation, we show that the observability of the wave equation in any dimension of space can be improved by allowing the domain of observation to move.
- In [57] we consider the controllability problem for finite-dimensional linear autonomous control systems with nonnegative controls. Despite the Kalman condition, the unilateral nonnegativity control constraint may cause a positive minimal controllability time. When this happens, we prove that, if the matrix of the system has a real eigenvalue, then there is a minimal time control in the space of Radon measures, which consists of a finite sum of Dirac impulses. When all eigenvalues are real, this control is unique and the number of impulses is less than half the dimension of the space. We also focus on the control system corresponding to a finite-difference spatial discretization of the one-dimensional heat equation with Dirichlet boundary controls, and we provide numerical simulations.

Let us also mention t the book chapter [31], which has been published this year.

6.5. Optimal control: new results

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

- In order to determine the optimal strategy to run a race on a curved track according to the lane number, we introduce in [7] 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 types of track since different designs of tracks lead to straights of different lengths. In particular, we find that the tracks with shorter straights lead to better performances, while the double bend track with the longest straight leads to the worst performances and the biggest difference between lanes. Then for a race with two runners, we introduce a psychological interaction: there is an attraction to follow someone just ahead, but after being overtaken, there is a delay before any benefit from this interaction occurs. We provide numerical simulations in different cases. Overall, the results agree with the IAAF rules for lane draws in competition, where the highest ranked athletes get the center lanes, the next ones the outside lanes, while the lowest ranked athletes get the inside lanes.
- 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 [11] 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 [15] we are concerned about the controllability of a general linear hyperbolic system 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 under some is a generic setting. We also present examples which yield that the generic requirement is necessary. Our approach is based on the backstepping method paying a special attention on the construction of the kernel and the selection of controls.
- A new approach to estimate traffic energy consumption via traffic data aggregation in (speed,acceleration) probability distributions is proposed in [18]. 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.
- In [24] we consider a spectral optimal design problem involving the Neumann traces of the Dirichlet-Laplacian eigenfunctions on a smooth bounded open subset Ω of $\mathbf{R}^n$. The cost functional measures the amount of energy that Dirichlet eigenfunctions concentrate on the boundary and that can be recovered with a bounded density function. We first prove that, assuming a L^1 constraint on densities, the so-called *Rellich functions* maximize this functional.Motivated by several issues in shape optimization or observation theory where it is relevant to deal with bounded densities, and noticing that the L^∞-norm of *Rellich functions* may be large, depending on the shape of Ω, we analyze the effect of adding pointwise constraints when maximizing the same functional. We investigate the optimality of *bang-bang* functions and *Rellich densities* for this problem. We also deal with similar issues for a close problem, where the cost functional is replaced by a spectral approximation. Finally, this study is completed by the investigation of particular geometries and is illustrated by several numerical simulations.
- In [25] we consider the task of solving an aircraft trajectory optimization problem where the system dynamics have been estimated from recorded data. Additionally, we want to avoid optimized trajectories that go too far away from the domain occupied by the data, since the model validity is not guaranteed outside this region. This motivates the need for a proximity indicator between a given trajectory and a set of reference trajectories. In this presentation, we propose such an indicator based on a parametric estimator of the training set density. We then introduce it as a penalty term in the optimal control problem. Our approach is illustrated with an aircraft minimal consumption problem and recorded data from real flights. We observe in our numerical results the expected trade-off between the consumption and the penalty term.
- In [36] we study how bad can be the singularities of a time-optimal trajectory of a generic control affine system. In the case where the control is scalar and belongs to a closed interval it was recently shown that singularities cannot be, generically, worse than finite order accumulations of Fuller points, with order of accumulation lower than a bound depending only on the dimension of the manifold where the system is set. We extend here such a result to the case where the control has an even number of scalar components and belongs to a closed ball.
- In [38] we develop a geometric analysis and a numerical algorithm, based on indirect methods, to solve optimal guidance of endo-atmospheric launch vehicle systems under mixed control-state constraints. Two main difficulties are addressed. First, we tackle the presence of Euler singularities by introducing a representation of the configuration manifold in appropriate local charts. In these local coordinates, not only the problem is free from Euler singularities but also it can be recast as an optimal control problem with only pure control constraints. The second issue concerns the

initialization of the shooting method. We introduce a strategy which combines indirect methods with homotopies, thus providing high accuracy. We illustrate the efficiency of our approach by numerical simulations on missile interception problems under challenging scenarios.

- We introduce and study in [51] the turnpike property for time-varying shapes, within the viewpoint of optimal control. We focus here on second-order linear parabolic equations where the shape acts as a source term and we seek the optimal time-varying shape that minimizes a quadratic criterion. We first establish existence of optimal solutions under some appropriate sufficient conditions. We then provide necessary conditions for optimality in terms of adjoint equations and, using the concept of strict dissipativity, we prove that state and adjoint satisfy the measure-turnpike property, meaning that the extremal time-varying solution remains essentially close to the optimal solution of an associated static problem. We show that the optimal shape enjoys the exponential turnpike property in term of Hausdorff distance for a Mayer quadratic cost. We illustrate the turnpike phenomenon in optimal shape design with several numerical simulations.
- The work [52] proposes a new approach to optimize the consumption of a hybrid electric vehicle taking into account the traffic conditions. The method is based on a bi-level decomposition in order to make the implementation suitable for online use. The offline lower level computes cost maps thanks to a stochastic optimization that considers the influence of traffic, in terms of speed/acceleration probability distributions. At the online upper level, a deterministic optimization computes the ideal state of charge at the end of each road segment, using the computed cost maps. Since the high computational cost due to the uncertainty of traffic conditions has been managed at the lower level, the upper level is fast enough to be used online in the vehicle. Errors due to discretization and computation in the proposed algorithm have been studied. Finally, we present numerical simulations using actual traffic data, and compare the proposed bi-level method to a deterministic optimization with perfect information about traffic conditions. The solutions show a reasonable over-consumption compared with deterministic optimization, and manageable computational times for both the offline and online parts.
- An extension of the bi-level optimization for the energy management of hybrid electric vehicles (HEVs) proposed in [52] to the eco-routing problem is presented in [53]. Using the knowledge of traffic conditions over the entire road network, we search both the optimal path and state of charge trajectory. This problem results in finding the shortest path on a weighted graph whose nodes are (position, state of charge) pairs for the vehicle, the edge cost being evaluated thanks to the cost maps from optimization at the 'micro' level of a bi-level decomposition. The error due to the discretization of the state of charge is proven to be linear if the cost maps are Lipschitz. The classical A^* algorithm is used to solve the problem, with a heuristic based on a lower bound of the energy needed to complete the travel. The eco-routing method is validated by numerical simulations and compared to the fastest path on a synthetic road network.
- In [58] we study a driftless system on a three-dimensional manifold driven by two scalar controls. We assume that each scalar control has an independent bound on its modulus and we prove that, locally around every point where the controlled vector fields satisfy some suitable nondegeneracy Lie bracket condition, every time-optimal trajectory has at most five bang or singular arcs. The result is obtained using first-and second-order necessary conditions for optimality.

COMMANDS Project-Team

7. New Results

7.1. Stochastic control and HJB equations

7.1.1. Monotone and second order consistent schemes for the Pucci and Monge-Ampere equations

In [9] we introduce a new strategy for the design of second-order accurate discretiza-tions of non-linear second order operators of Bellman type, which preserves degenerate ellipticity. The approach relies on Selling's formula, a tool from lattice geometry, and is applied to the Pucci and Monge-Ampere equations, discretized on a two dimensional cartesian grid. In the case of the Monge-Ampere equation, our work is related to both the stable formulation and the second order accurate scheme. Numerical experiments illustrate the robustness and the accuracy of the method.

7.1.2. Mean-field games of control

In [3], an existence result for a class of mean field games of controls is provided. In the considered model, the cost functional to be minimized by each agent involves a price depending at a given time on the controls of all agents and a congestion term. The existence of a classical solution is demonstrated with the Leray–Schauder theorem; the proof relies in particular on a priori bounds for the solution, which are obtained with the help of a potential formulation of the problem.

7.2. Optimal control of PDEs

7.2.1. Optimal Control of an Age-Structured System with State Constraints

In [10] we study an optimal control problem with state constraints where the state is given by an age-structured, abstract parabolic differential equation. We prove the existence and uniqueness of solution for the state equation and provide first and second parabolic estimates. We analyze the differentiability of the cost function and, based on the general theory of Lagrange multipliers, we give a first order optimality condition. We also define and analyze the regularity of the costate. Finally, we present a pregnancy model, where two coupled age-structured equations are involved, and we apply the obtained results to this case.

7.2.2. Feedback laws

The articles [4], [5], [6], co-written by L. Pfeiffer in the framework of his former position at the University of Graz, deal with the computation of feedback laws for stabilization problems of PDE systems. These problems are formulated as infinite-horizon optimal control problems.

In [5], we prove that the value function associated with bilinear stabilization problems (including some control problems of the Fokker-Planck equation) can be expanded as a Taylor expansion, where the second-order term is the solution to an algebraic Riccati equation and where the terms of order three and more are solutions to well-posed linear equations. These equations are obtained by successive differentiation of the HJB equation. A polynomial feedback law can be deduced from the Taylor approximation and its efficiency is analyzed. This approach generalizes the classical LQR-stabilization method.

In [4], we apply the methodology previously described to a stabilization problem of the 2D Navier-Stokes equation. Numerical results are provided.

In [6], we analyze an implementation of the Receding-Horizon Control method utilizing the Taylor expansion of the value function as a terminal cost. More precisely, we show that the method converges at an exponential rate with respect to the prediction horizon and the degree of the Taylor approximation.

7.3. Energy management for hybrid vehicles

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

In [7], a new approach to estimate traffic energy consumption via traffic data aggregation in (speed,acceleration) probability distributions is proposed. 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.

7.3.2. A bi-level energy management strategy for HEVs under probabilistic traffic conditions

In [11], we propose a new approach to optimize the consumption of a hybrid electric vehicle taking into account the traffic conditions. The method is based on a bi-level decomposition in order to make the implementation suitable for online use. The offline lower level computes cost maps thanks to a stochastic optimization that considers the influence of traffic, in terms of speed/acceleration probability distributions. At the online upper level, a deterministic optimization computes the ideal state of charge at the end of each road segment, using the computed cost maps. Since the high computational cost due to the uncertainty of traffic conditions has been managed at the lower level, the upper level is fast enough to be used online in the vehicle. Errors due to discretization and computation in the proposed algorithm have been studied. Finally, we present numerical simulations using actual traffic data, and compare the proposed bi-level method to a deterministic optimization with perfect information about traffic conditions. The solutions show a reasonable over-consumption compared with deterministic optimization, and manageable computational times for both the offline and online parts.

7.3.3. An Eco-routing algorithm for HEVs under traffic conditions

In [12], an extension of the bi-level optimization for the energy management of hybrid electric vehicles (HEVs) proposed above to the eco-routing problem is presented. Using the knowledge of traffic conditions over the entire road network, we search both the optimal path and state of charge trajectory. This problem results in finding the shortest path on a weighted graph whose nodes are (position, state of charge) pairs for the vehicle, the edge cost being evaluated thanks to the cost maps from optimization at the 'micro' level of a bi-level decomposition. The error due to the discretization of the state of charge is proven to be linear if the cost maps are Lipschitz. The classical $A*$ algorithm is used to solve the problem, with a heuristic based on a lower bound of the energy needed to complete the travel. The eco-routing method is validated by numerical simulations and compared to the fastest path on a synthetic road network.

DISCO Project-Team

5. New Results

5.1. Multiplicity-induced-dominancy

Participants: Islam Boussaada, Guilherme Mazanti, Hugues Mounier [L2S, CentraleSupélec], Silviu-Iulian Niculescu.

The effects of multiplicity of spectral values on the exponential stability of reduced-order retarded differential equation were emphasized in recent works. In [13] the general class of second-order retarded differential equations is studied. A parametric multiplicity-induced-dominancy (MID) property is characterized, allowing a delayed stabilizing design with reduced complexity. The proposed approach is merely a delayed-output-feedback where the candidates' delays and gains result from the manifold defining the maximal multiplicity of a real spectral value, then, the dominancy is shown using the argument principle.

The work [52] considers retarded differential equations of arbitrary order with a single delay. The existence of a real root with maximal multiplicity is characterized in terms of the equation parameters. This root is shown to be always strictly dominant, determining thus the asymptotic behavior of the system. The dominancy proof is based on improved a priori bounds on the imaginary part of roots on the complex right half-plane and a suitable factorization of the characteristic function, which is an alternative technique to the argument principle.

In [53] we extend the MID property to a given pair of complex conjugate roots for a generic second-order retarded differential equation. Necessary and sufficient conditions for the existence of such a pair are provided, and it is also shown that such a pair is always necessarily dominant. It appears also that when the frequency corresponding to this pair of roots tends to 0, then the pair of roots collapse into a real root of maximal multiplicity. The latter property is exploited in the dominancy proof together with a study of crossing imaginary roots.

In [41] a control-oriented model of torsional vibrations occurring in rotary drilling process is proposed. More precisely, a wave equations with weak damping term is considered. An appropriate stabilizing controller with a reduced number of parameters is proposed for damping such torsional vibrations. Such a controller allows to further explore the effect of multiple roots with maximal admissible multiplicity for linear neutral system with a single delay.

5.2. Pole placement techniques for time-delay systems

Participants: Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S, CentraleSupélec], Fazia Bedouhene [University Mouloud Mammeri de Tizi Ouzou, Algeria].

The interest in investigating multiple roots does not rely on the multiplicity itself, but rather on its connection with the dominance of this root, and the corresponding applications in stability analysis and control design. The work [31] extends the analytical characterization of the spectral abscissa for retarded time-delay system with real spectral values which are not necessarily multiple. The effect of the coexistence of such non oscillatory modes on the asymptotic stability of the trivial solution is explored. In particular, the coexistence of an appropriate number of real spectral values makes them rightmost-roots of the corresponding quasipolynomial. Furthermore, if they are negative, this guarantees the asymptotic stability of the trivial solution. As an application of the proposed rightmost-characteristic root assignment, the problem of the vibration damping for a thin flexible beam is considered in [33]. The considered beam is equipped with two piezoelectric patches: one of them works as a sensor and the other as an actuator. Each one of them is bonded on one side of the beam and both are collocated. The model of this system is obtained numerically thanks to a finite element modeling, leading to a linear state-space model. The design of a controller based on proportional and delayed-proportional actions on the input and output signals is proposed, where the properties of the proposed output feedback controller in terms of vibration damping and of robustness is discussed.

5.3. PID tuning for controlling delayed dynamics

Participants: Jie Chen [City University of Hong Kong], Jianqi Chen [City University of Hong Kong], Andong Liu [City University of Hong Kong], Dan Ma [Northeastern University, China], Silviu Niculescu.

Nowadays, the PID controller is the most used in controlling industrial processes. In [21] such a controller is further explored in the control of delayed dynamics. An explicit lower bound on the delay margin of second-order unstable delay systems achievable by PID control is established, which provides a priori a guaranteed range of delay values over which a second-order delay plant can be stabilized by a PID, and more generally, a finite-dimensional LTI controller. This is done by deriving lower bounds on the delay margin achievable by PD controllers, whereas this margin constitutes a lower bound on that achievable by PID controllers. Analysis shows that in most cases our results can be significantly less conservative than the lower bounds obtained elsewhere using more sophisticated, general LTI controllers.

5.4. Frequency-sweeping techniques in delayed dynamics analysis

Participants: Arben Cela [ESIEE Paris], Xu-Guang Li [Northeastern University, China], Xu Li [Northeastern University, China], Jiang-Chian Li [Northeastern University, China], Zhi-Zhong Mao [Shenyang University], Silviu Niculescu, Lu Zhang [Shenyang University].

The stability of linear systems with multiple (incommensurate) delays is investigated in [20], by extending a recently proposed frequency-sweeping approach. First, we consider the case where only one delay parameter is free while the others are fixed. The complete stability w.r.t. the free delay parameter can be systematically investigated by proving an appropriate invariance property. Next, we propose an iterative frequency-sweeping approach to study the stability under any given multiple delays. Moreover, we may effectively analyze the asymptotic behavior of the critical imaginary roots (if any) w.r.t. each delay parameter, which provides a possibility for stabilizing the system through adjusting the delay parameters. The approach is simple (graphical test) and can be applied systematically to the stability analysis of linear systems including multiple delays. A deeper discussion on its implementation is also proposed. Finally, various numerical examples complete the presentation.

In most of the numerical examples of time-delay systems proposed in the literature, the number of unstable characteristic roots remains positive before and after a multiple critical imaginary root (CIR) appears (as the delay, seen as a parameter, increases). This fact may lead to some misunderstandings: (i) A multiple CIR may at most affect the instability degree; (ii) It cannot cause any stability reversals (stability transitions from instability to stability). As far as we know, whether the appearance of a multiple CIR can induce stability is still unclear (in fact, when a CIR generates a stability reversal has not been specifically investigated). In [19], we provide a finer analysis of stability reversals and some new insights into the classification: the link between the multiplicity of a CIR and the asymptotic behavior with the stabilizing effect. Based on these results, we present an example illustrating that a multiple CIR's asymptotic behavior is able to cause a stability reversal. To the best of the authors' knowledge, such an example is a novelty in the literature on time-delay systems.

The work [30] focuses on the stability property of a class of distributed delay systems with constant coefficients. More precisely, we will discuss deeper the stability analysis with respect to the delay parameter. Our approach will allow to give new insights in solving the so-called complete stability problem. There are three technical issues need to be studied: First, the detection of the critical zero roots; second, the analysis of the asymptotic behavior of such critical zero roots; third, the asymptotic behavior analysis of the critical imaginary roots with respect to the infinitely many critical delays. We extended our recently-established frequency-sweeping approach, with which these technical issues can be effectively solved. More precisely, the main contributions of this paper are as follows: (i) Proposing a method for the detection of the critical zero roots. (ii) Proposing an approach for the asymptotic behavior analysis of such critical zero roots. (iii) The invariance property for the critical imaginary roots can be proved. Based on these results, a procedure was proposed, with which the complete stability analysis of such systems was accomplished systematically. Moreover, the procedure represents a unified approach: Most of the steps required by the complete stability problem may be fulfilled through observing the frequency-sweeping curves. Finally, some examples illustrate the effectiveness and advantages of the approach.

5.5. Weierstrass approach to asymptotic behavior of retarded differential equations

Participants: Jie Chen [City University of Hong Kong], Liliana Felix [University of San Luis Potosi], Alejandro Martinez-Gonzalez, Cesar F. Mendez-Barrios [University of San Luis Potosi], Silviu Niculescu.

The work [22] focuses on the analysis of the behavior of characteristic roots of time-delay systems, when the delay is subject to small parameter variations. The analysis is performed by means of the Weierstrass polynomial. More specifically, such a polynomial is employed to study the stability behavior of the characteristic roots with respect to small variations on the delay parameter. Analytic and splitting properties of the Puiseux series expansions of critical roots are characterized by allowing a full description of the cases that can be encountered. Several numerical examples encountered in the control literature are considered to illustrate the effectiveness of the proposed approach.

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

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

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 [59] and analyzed carefully the position of the poles of such systems in the right half-plane. We have considered delay systems with characteristic equation being a quasi-polynomial with one delay and polynomials of degree one. It is shown that for a subclass of systems which have a chain of poles clustering the imaginary axis by the left, the procedure of Walton and Marshall fails: we prove the existence, for an infinitesimally small delay, of a positive real pole at infinity. This real pole is then proved to be the unique pole of the system in the closed right half-plane for all values of the delay. Some numerical examples illustrate the results [39]. We are currenlty extending those results to the general case of polynomials of degree $n > 1$.

5.7. $L2$ and BIBO Stability of systems with variable delays

Participants: Catherine Bonnet, Jonathan R. Partington [Univ of Leeds,U.K.].

There has been a growing interest in systems with time-varying delays in recent years and to the best of our knowledge, no study has been made of the input–output stability of a standard feedback scheme involving a system with time-varying delays. We have considered two versions of input–output stability: so-called Hinfinity and BIBO-stability. Retarded and neutral type systems with pointwise or distributed delays are studied here. We perform a stability analysis and discuss feedback stabilization. The results we derive yield very explicit estimates for stability margins [40].

5.8. Stability Analysis of Linear Partial Differential Equations

Participants: Giorgio Valmorbida, Aditya Gahlawat [University of Illinois at Urbana-Champaign].

We proposed a method to perform stability analysis of one-dimensional Partial Integro-Differential Equations. The relevance of the proposed results lies on the fact that we cast the Lyapunov inequalities as a differential inequality in two dimensions. The proposed structure for the inequalities is motivated by the same structure as the one used in the study of backstepping feedback laws, a successful strategy applied for several one-dimensional PDE systems. The advantage of the proposed Lyapunov analysis can be studied in a simpler manner as well as the fact that the backstepping law can be approximated by simpler laws and the stability can still be studied trhough the solution to the set of proposed inequalities.

We rely on Lyapunov analysis to establish the exponential stability of the systems. Then we present a test for the verification of the underlying Lyapunov inequalities, which relies on the existence of solutions of a system of coupled differential equations.

We illustrate the application of this method in several examples of PDEs defined by polynomial data, we formulate a numerical methodology in the form of a convex optimization problem which can be solved algorithmically. We show the effectiveness of the proposed numerical methodology using examples of different types of PDEs.

We are currently studying the extensions of coupled PDE-ODE systems.

5.9. Stability analysis of Piece-Wise Affine Systems

Participants: Giorgio Valmorbida, Leonardo Broering Groff, Joao Manoel Gomes Da Silva Jr [Universidade Federal do Rio Grande do Sul].

Piece-wise affine systems appear when linear dynamics are defined in different partitions of the state space. This type of system naturally appears whenever actuators have different stages or saturate or whenever non-linear control laws are obtained as the solution to a parameterised optimization problem as, for instance for systems with feedback laws based on the so-called explicit Model Predictive Control. Even though the dynamics is simple to describe, the stability analysis, performance assessment and robustness analysis are difficult to perform since, due to the often used explicit representation, the Lyapunov stability and dissipation tests are often described in terms of a number of inequalities that increase exponentially on the number of sets in the partition. Moreover regional stability and uncertainties corresponding to modification on the partition are difficult to study in this scenario.

To overcome these difficulties we have proposed an implicit representation for this class of systems in terms of ramp functions. The main advantage of such a representation lies on the fact that the ramp function can be exactly characterized in terms of linear inequalities and a quadratic equation, namely a linear complementarity condition. Thanks to the characterization of the ramp function and the implicit description of the PWA system the verification of Lyapunov inequalities related to piecewise quadratic functions can be cast as a pair of linear matrix inequalities.

The obtained formulation opens several possibilities to study the class of piecewise affine systems and their robustness properties. Indeed the fact that some partitions are uncertain is more easily coped with the proposed approach as they are described as parametric uncertainties of the implicit representation. Also, systems of larger dimension can be studied.

The stability analysis of the particular subclass of systems given by asymmetric saturation can also be performed with discontinuous Lyapunov functions for discrete-time systems.

5.10. Set Invariance for Descriptor Systems

Participants: Giorgio Valmorbida, Ye Wang [Universidade Federal do Rio Grande do Sul], Sorin Olaru [L2S, CentraleSupélec], Vicenç Puig [Universitat Politècnica de Catalunya], Gabriela Cembrano [Universitat Politècnica de Catalunya].

Some descriptor systems, characterized by a difference-algebraic relation, appear in economic systems. For such a class of systems we study robust invariant set characterizations of discrete-time descriptor systems and propose an active mode detection mechanism. The considered class of descriptor systems assumes regularity, stability and is affected by unknown-but-bounded disturbances.

As a first theoretical result, we establish a general framework for robust invariant sets for discrete-time descriptor systems in both causal and non-causal cases. Particular transformations are subsequently proposed for handling causal and non-causal descriptor systems and will be used to characterize the effects of disturbances. Based on these set-theoretic notions and a designed input signal for active set separations, we propose an active mode detection mechanism by exploiting the strong invariance properties.

5.11. New advances on backstepping

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Laurent Burlion [Rutgers Univ.].

We worked on the problem of improving a major control design technique for nonlinear continuous-time systems called backstepping by using a fundamentally new approach which uses as key ingredient the introduction in the control of artificial delays or the use of dynamic extensions.

In the paper [24], we adopted a technique which is based on the introduction of pointwise delays (and not of distributed terms) to solve a challenging input-to-state stabilization problem for a chain of saturated integrators when the variables are not accurately measured. Let us observe that classical backstepping does not apply in the considered case.

In the paper [23], we constructed bounded globally asymptotically stabilizing output feedbacks for a family of nonlinear systems, using a dynamic extension and a converging-input-converging-state assumption. We provided sufficient conditions for this assumption to hold, in terms of Lyapunov functions. The novelty is that our construction provides formulas for the control bounds while allowing uncertainties that prevent the use of classical backstepping in cases where only part of the state variable is available. We illustrated our work with an engineering application: the single-link direct-drive manipulator.

5.12. Finite time observers

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Saeed Ahmed [University of Kaiserslautern, Germany], Thach Dinh [CNAM], Tarek Raissi [CNAM].

Finite time observers are remarkably efficient when the value of the state is needed in a short time. By contrast with them, the solutions asymptotic observers may take a long time to be close to the solutions of the studied systems and may exhibit large transient errors. Motivated by this general fact, we produced three works.

In the work [12], we proposed finite time observers for time-varying nonlinear systems with delays in the outputs. When disturbances are present, we provide approximate values for the solutions which are expressed as upper bounds on the approximation errors after a suitable finite time. We illustrated our work via systems arising in the study of vibrating membranes, where time-varying coefficients can be used to represent intermittent measurements.

In paper [36], we use finite time reduced order continuous-discrete observers to solve an output feedback stabilization problem for a broad class of nonlinear systems whose output contains uncertainty. Unlike earlier works, our feedback control is discontinuous, but it does not contain any distributed terms, which is an advantage because the implementation of these terms may cause instability. We illustrated our main result by applying it to design a dynamic output feedback to solve a tracking problem for nonholonomic systems in chained form.

The paper [35] is devoted to the construction of finite time observers for discrete-time systems. We developped a new technique, which uses past values of the output. We considered the case where the systems are affected by additive disturbances and disturbances in the output. Exact estimation or approximate estimation have been achieved, depending on the absence or the presence of unknown but bounded uncertainties, respectively.

5.13. Observers with discrete measurements

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Saeed Ahmed [University of Kaiserslautern, Germany].

We studied the important case where the measurements of a system are discrete because output of this type may preclude the use of observers designed under the assumption that the measurements are continuous.

In the paper [25], we have studied time-varying linear systems in the difficult case where the inputs and outputs have sampling and delays, and where the systems and outputs contain uncertainties. The observers we have proposed are of continuous-discrete type and have no distributed terms. We allowed the delays to be arbitrarily large and proved that the observer in combination with a linear control result in an input-to-state stability, under delays and sampling. We illustrated our work in two examples including a DC motor model.

In the work [38], we have revisited a well-known contribution of observer design for continuous-time systems with discrete measurements which relies on a dynamic extension. Using a stability analysis which relies on the recent technique called "trajectory based approach", we proved that, for systems with asynchronous sampling, the proposed dynamic observer is converging even when the size of some (sufficiently scarce) intervals between 2 measurements is larger than the upper bound ensuring convergence of the observer that is provided in the literature. A scarcety condition on these intervals is exhibited.

5.14. Observer for a rigid body

Participants: Frédéric Mazenc, Maruthi Akella [University of Texas, USA], Hongyang Duong [Harbin Institute of Technology], Qinglei Hu [Beihang University].

In the work [15], observers are proposed for models of rigid bodies in the case where only a part of the state variables can be measured. The design is based on the dual-quaternion description. To achieve tracking control objectives, the proposed observer are combined 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. Almost global asymptotic stability of the closed-loop dynamics is guaranteed. We performed numerical simulations for a prototypical spacecraft pose tracking mission application to illustrate the effectiveness and robustness of the proposed method.

5.15. Systems with pointwise delays

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Robledo Gonzalo [Univ. de Chile, Chile], Silviu Niculescu.

Frequently, the presence of delays is an obstacle to the stability analysis or the control of systems. Two of our works originate in the will to overcome this obstacle, in two distinct contexts.

The contribution [26] is devoted to the study of a model of a chain of two bio-reactors called 'chemostats'. One contains two microbial species in competition for a single limiting nutrient and receives an external input of the less advantaged competitor, which is cultivated in the other one. Pointwise delays are present. Under a condition on their size, we obtained sufficient conditions ensuring coexistence of all the species in competition. To prove the result, we adopted a Lyapunov based technique.

The contribution of [37] is twofold. In a first part, we exhibited a fundamental feature of the systems with a pointwise periodic time-varying delay: we have shown by a counterexample that the asymptotic stability of such a system cannot be deduced from the average value of the delay (even when the delay is 'rapidly' varying). In a second part, motivated by this counterexample, we proposed a new representation of systems with time-varying delays, which is helpful to carry out stability analyses and to develop a new state feedback stabilization method.

5.16. Control of an aircraft

Participants: Frédéric Mazenc, Michael Malisoff [LSU], Laurent Burlion [Rutgers Univ.].

The work [34] adapts some ideas we published in previous contributions to a control problem for a chain of saturating integrators for dynamics with outputs that occurs in the vision based landing of aircraft. The major obstacle that we overcome is due to the fact that only imprecise output measurements are available. The control laws we designed are bounded by an arbitrarily small constant. The closed-loop systems we obtained possess the robustness property called "local input-to-state stability".

5.17. Effect of environment on population dynamics

Participants: Islam Boussaada, Silviu Niculescu, Jun-Xiu Chen [Nothestern University], Sette Diop [L2S, CentraleSupélec], Xu-Guang Li [Nothestern University], Paul Raynaud de Fitte [LMRS, Université de Rouen Normandie], Safia Slimani [LMRS, Université de Rouen Normandie], Sami Tliba [L2S, CentraleSupélec].

Competition in population dynamics is often considered to be governed by predator-prey models. In particular, Lotka-Volterra models are intensively used in this context.

A modified version of a prey-predator system with Leslie-Gower and Holling type II functional responses incorporating a refuge for preys is studied in [27]. Such a refuge substantially complicates the dynamics of the system. We study the local and global dynamics and the existence of limit-cycles. We also investigate conditions for extinction or existence of a stationary distribution, in the case of a stochastic perturbation of the system.

Most of the reported Lotka-Volterra examples have at most one stability interval for the delay parameters. Furthermore, the existing methods fall short in treating more general case studies. Inspired by some recent results for analyzing the stability of time-delay systems, this paper focuses on a deeper characterization of the stability of Lotka-Volterra systems w.r.t. the delay parameters. In [58], we introduced the recently-proposed frequency-sweeping approach to study the complete stability problem for a broad class of linearized Lotka-Volterra systems. As a result, the whole stability delay-set is analytically determined. Moreover, as a significant byproduct of the proposed approach, some Lotka-Volterra examples are found to have multiple stability delay-intervals. In some situations, a longer maturation period of species is helpful for the stability of a population system.

In another context, the effect of environment on yeast population dynamics is studied in [28]. In presence of oxygen cells usually adopt efficient metabolism in order to maximize energy production yield in poor diet. If nutrient resource increases, a metabolic shift from efficient metabolism (respiration) to inefficient metabolism (fermentation) is reflecting a minimal cost principle of living systems to optimize fitness. This is known as the Crabtree/Warburg effect. A model that describes the population dynamics of cells and the input growth condition is established. Proof of principle has been constructed using a battery of growth experiments on Crabtree-positive yeasts–Saccharomyces under various conditions of glucose in aerobic and micro-aerobic conditions. General cell growth model estimating metabolic shift has been constructed based on an Auto-Regressive approach.

5.18. Distributed Algorithms for Microbiological systems

Participants: Lotfi Baour, Catherine Bonnet, Da-Jung Cho, Walid Djema [BIOCORE project team], Lucas Leclerc, Matthias Fuegger [MEXICO project team], Frédéric Mazenc, Tomas Nowak [LRI, Univ Paris-Sud], Cristina Stoica [CentraleSupélec].

This project led by M. Fuegger and T. Nowak considers microbiological distributed systems such as bacterial cultures. Our goal is to develop algorithms to be used in such low-powered biological computing systems. We have considered a distributed computation model where bacteria communicate via concentrations of small signaling molecules. Algorithms designed for such a model are of importance to provide services like clock synchronization. Basic ODE models for well-mixed solutions are readily available from systems biology. This year, we have paid attention to ODE and PDE models presented in [56], [55]. We have analyzed the influence of model parameters on the stability of the system. Moreover, looking at the involved basic biochemical reactions we have considered some changes in the modelling.

FACTAS Project-Team

6. New Results

6.1. Inverse problems for Poisson-Laplace equations

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

6.1.1. Inverse magnetization issues from planar data

The overall goal is here 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 (thin sample) 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.

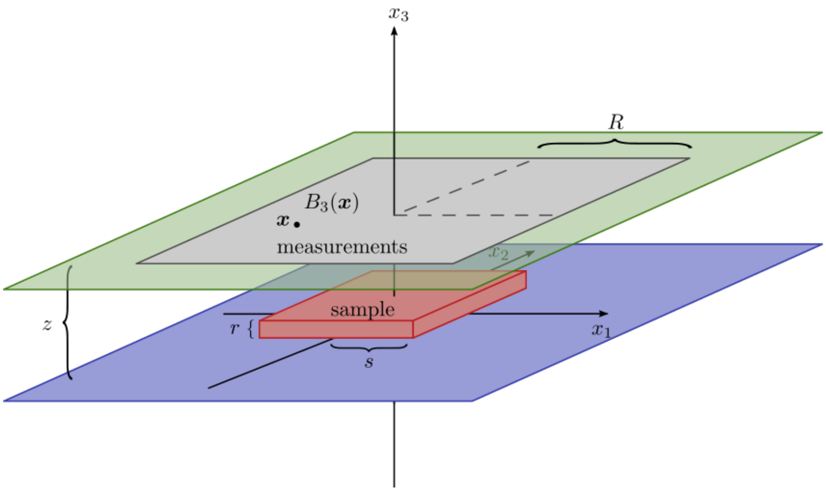


Figure 3. Schematic view of the experimental setup

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 investigation of the recovery of magnetizations modeled by signed measures on thin samples, and we singled out an interesting class that we call slender samples. These are sets of zero measure in $\mathbb{R}^3$, the complement of which has all its connected components of infinite measure. For such samples, we showed that consistent recovery is possible, in the Morozov discrepancy limit, by penalizing the total variation when either the support of the magnetization is purely 1-unrectifiable (which holds in particular for dipolar models) or the magnetization is unidirectional (an assumption of physical interest because igneous rocks acquire magnetization by cooling down in some ambient field). These notions play a role similar to sparsity in this infinite-dimensional context. An article has been published to report on these results [16]. Moreover, in the case of planar samples (which are certainly slender), a loop decomposition of divergence free measures was obtained, which sharpens in the 2-D setting the structure theorem of [77], and allowed us to prove, using in addition the real analyticity of the operators relating the magnetization to the field, 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 using a variant of the FISTA algorithm has been set up which yields promising results when measurements are carried out on a relatively large surface patch. 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.

We also continued investigating the recovery of the moment of a magnetization, an important physical quantity which is in principle easier to reconstruct than the full magnetization because it is simply a vector in $\mathbb{R}^3$ that only depends on the field (*i.e.* magnetizations that produce the zero field also have zero moment). For the case of thin samples, we published an article reporting the construction of linear estimators for the moment from the field, based on the solution of certain bounded extremal problems in the range of the adjoint of the forward operator [15]. On a related side, we also setup other linear estimators based on asymptotic results, in the previous years. These estimators are not limited to thin samples and can in principle estimate the net moment of 3D samples, provided that the dimensions of the sample are small with respect to the measurement area. Numerical experiments confirm that linear estimators (both kinds) make essential use of field values taken at the boundary of the measurement area, and are easily blurred by noise. We experimentally confirmed this sensitivity on a rather simple case: a small spherule has been magnetized in a controlled way by our partners at MIT, and its net moment has been measured by a classical magnetometer. The spherule has then been measured with the SQUID microscope, with several choices for important parameters (height of the sensor with respect to the spherule, sensitivity of the instrument, size of the 2D rectangle on which measurements are performed, size of the sample step). We applied our (asymptotics based) linear estimator on these experimental maps and they turn out to be clearly affected, especially when the data at the edges of the map are involved. The nature of the noise due to the microscope itself (electronic and quantization noise) might play an important role, as it is known to be non-white, and therefore can affect our methods which sum it up. Subsequently, we now envisage the possibility of modeling the structure of the noise to pre-process the data.

Finally, 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, we set up some best approximation issues related to inverse recovery and relevant BEP problems in Hardy classes of holomorphic functions, see Section 3.3.1 and [25], which is joint work with E. Pozzi (Department of Mathematics and Statistics, St Louis Univ., St Louis, Missouri, USA). 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.

6.1.2. Inverse magnetization issues from sparse cylindrical data

The team Factas was a partner of the ANR project MagLune on Lunar magnetism, headed by the Geophysics and Planetology Department of Cerege, CNRS, Aix-en-Provence, which ended this year (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 was 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.

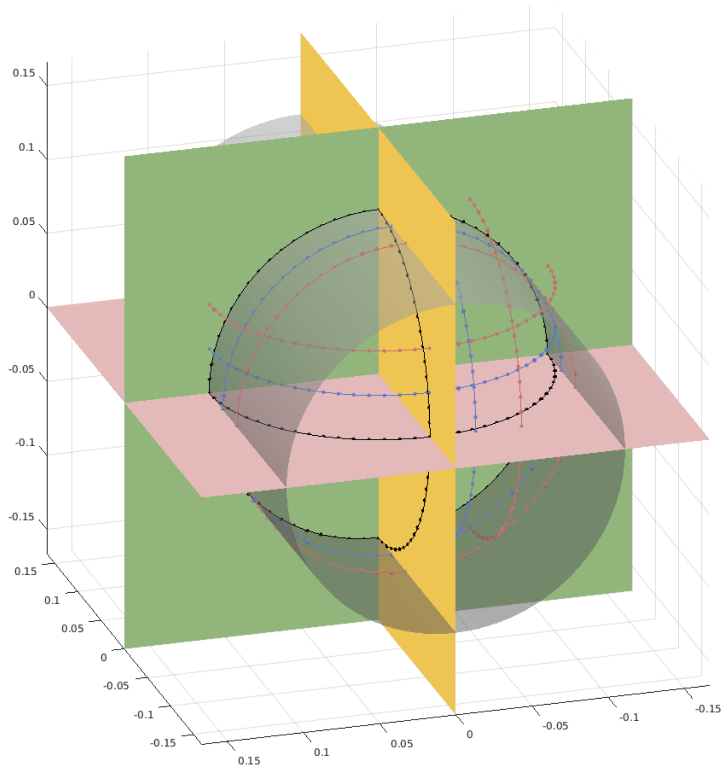


Figure 4. Typical measurements obtained with the instrument of Cerege. Measurements of the field are performed on nine circles, given as sections of three cylinders. On each circle, only one component of the field is measured: the component B_h along the axis of the corresponding cylinder (blue points),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

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 3.4.3 and 6.1.3), we try to recover the position and the moment of the dipole using the available measurements. This work, which is still ongoing, constitutes the topic of the PhD thesis of K. Mavreas, whose defense is scheduled on January 31, 2020. 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 the fact that, whatever component of the field is measured, the (square of the) measurements performed on the circle at height h correspond to a rational function of the form $p(z)/(z-u_h)^5$ where p is a polynomial of degree at most 4 and u_h is the complex number $u_h = \frac{1+\rho^2+(h-z)^2}{\rho}\, e^{i\phi}$. The numerator p depends on the moment of the dipole, on the height h and on the kind of component which is measured. In contrast, u_h can be estimated by rational approximation techniques, which allows one to obtain ϕ directly and gives the relation $\rho|u_h| = 1+\rho^2+(h-z)^2$. Combining the relations obtained at several heights, we proposed several methods to estimate ρ and z.

This year has been mostly devoted to running numerical experiments on synthetic examples. The first important observation is that the minimization criterion that we use to recover u_h can have local minima achieving very small values, and that can sometimes erroneously be considered as the global minimum. We started studying theoretically this phenomenon, see Section 6.7.1 . This means that the relative error $\varepsilon = |u_h - \widetilde{u_h}|/|u_h|$ between the theoretical minimum u_h and the value $\widetilde{u_h}$ estimated by our algorithm can vary from almost 0 to more than 50%, even when the data used as measurements exactly correspond to the field produced by a magnetic dipole. The second important observation is that the statistical distribution of ε (when the position of the dipole is uniformly chosen within a cylinder with a moment uniformly chosen on the unit sphere) depends on the measured component of the field. Figure 5 shows the distribution experimentally observed. The vertical component of the field noticeably leads to better estimates for u_h than both other components. The third important observation that we made is that the presence of noise on the measurements, even moderate, significantly alters the quality of the estimation of u_h. Figure 6 shows the distribution experimentally observed in the same conditions as before, but using data contaminated with a random normal noise with standard deviation 5% of the maximal absolute value of the measured component.

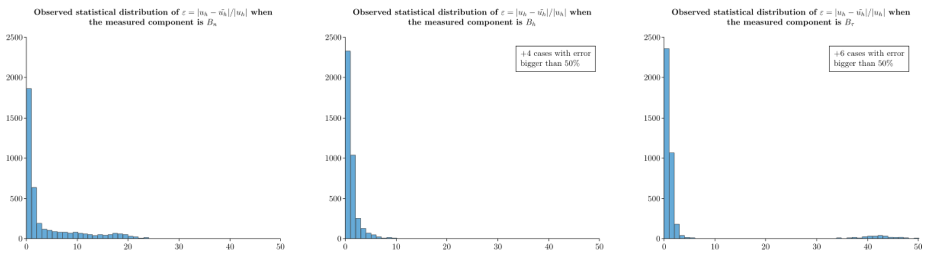


Figure 5. Different statistical behavior of the error of the recovered pole position, depending on the measured component of the field. Each bar indicates the number of cases observed with an error within the range of abscissas of the bar. The experiment has been performed with 4000 dipoles whose position and moment were randomly chosen (uniformly inside a cylinder, and on the unit sphere, respectively).

These observations are somehow bad news, as the method we propose is based on recovering the position of the dipole by using the values u_h collected at several heights h. However, our experiments also revealed an unexpected good news: while the estimation of u_h itself is often bad, as soon as the data are not perfect, its argument (from which ϕ is immediately deduced) turns out to be fairly well recovered. This is illustrated in Figure 7 which shows, on the set of experiments of Figure 6 , the position of the 4000 dipoles, with a color indicating whether ε is big (left part of the figure) and whether the error on the argument of u_h is big (right part of the figure). As can be seen, the angular error is most of the time smaller than $10°$, even for dipoles

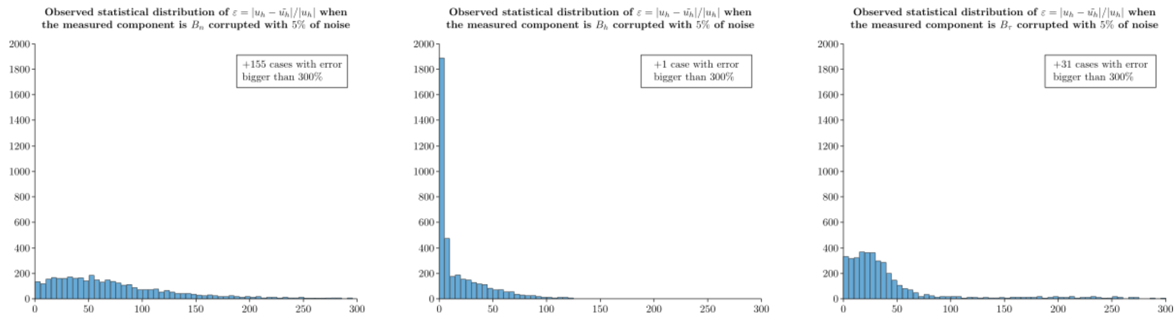


Figure 6. Statistical behavior of the error of the recovered pole position, when the measurement are corrupted with a centered Gaussian noise with standard deviation 5% *of the maximal absolute value of the measured component. The setup is otherwise the same as in Figure 5 .*

for which ε is fairly big. This phenomenon is probably due to the fact that local minima of the criterion tends to have a complex argument close to the complex argument of the global minimum, a phenomenon that we started to study theoretically (see Section 6.7.1).

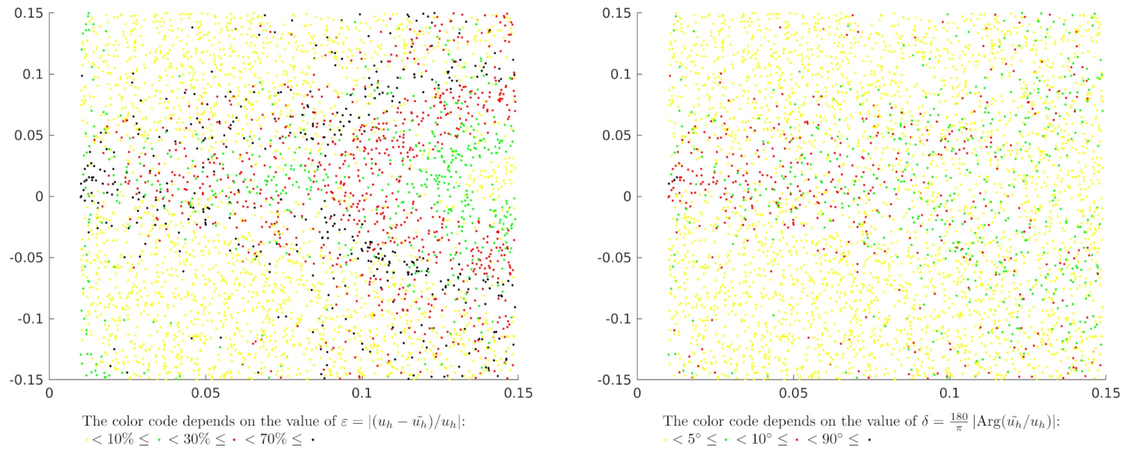


Figure 7. Each dot corresponds to the position of a dipole of the set of experiments described in Figure 6 . What is shown is indeed (ρ, z) *where* ρ *and* z *correspond to, respectively, the radial distance and height of the dipole position, expressed in cylindrical coordinates. The position is displayed with a dot whose color indicates the order of magnitude of the modulus of the relative error (figure on the left) and of the angle error (figure on the right) committed in the recovery of the value* u_h*.*

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 [8], [42] 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 3.4.3) is being developed, in collaboration with the Inria team Athena and the CMA - Mines ParisTech. Its Matlab version now incorporates the treatment of MEG data, the aim being to handle simultaneous EEG–MEG recordings available from our partners at INS, hospital la Timone, Marseille. Indeed, it is now possible to use simultaneously EEG and MEG 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 enhances the accuracy of our source recovery algorithms. Note that FS3D takes as inputs actual EEG measurements, like time signals, and performs a suitable singular value decomposition in order to separate independent sources.

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 [9], there is no mathematical justification so far why multiple poles generate such strong accumulation of the poles of the approximants (see Section 6.7.1). 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).

This year, we started considering a different class of models, not necessarily dipolar, and related estimation algorithms. Such models may be supported on the surface of the cortex or in the volume of the encephalon. We represent sources by vector-valued measures, and in order to favor sparsity in this infinite-dimensional setting we use a TV (i.e. total variation) regularization term as in Section 6.1.1 . The approach follows that of [16] and is implemented through two different algorithms, whose convergence properties are currently being studied. Tests on synthetic data from a few dipolar sources provide results of different qualities that need to be better understood. In particular, a weight is being added in the TV term in order to better identify deep sources. This is the topic of the starting PhD research of P. Asensio and M. Nemaire. Ultimately, the results will be compared to those of FS3D and other available software tools.

6.2. Matching problems and their applications

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

6.2.1. Multiplexer synthesis via interpolation and common junction design

In the context of David Martinez Martinez’s PhD funded partly by CNES the synthesis of multiplexer responses was considered using multipoint matching techniques. Indeed, synthesizing the response of multiplexer composed of a set of channel filters connected via common manifold junction to a common port can be seen as a matrix version application of our multipoint matching result for filters [7]. For short a simultaneous matching solutions is sought for, where each channel filter matches the load it is connected at specified matching frequencies. The difficulty here is that the load seen by each filter, depends explicitly of the response of the other filters by means of the common junction’s response: the multiplexer synthesis problem is therefore, in general, strictly harder than the filter multipoint matching problem, and can’t be solved by a sequential solving of independent «scalar» problems. A notable exception to this statement is obtained when a totally decoupling common junction is considered. This somehow artificial situation was taken as a start of a continuation algorithm, during which the decoupling junction response is moved step by step via a linear trajectory towards the target junction while the simultaneous matching problem is solved all along via a differential predictor corrector method. Whereas all «accidents» of branch point type that can occur during this procedure are not classified yet, one major obstruction to the continuation process is the occurrence of manifold peaks. The latter are due to resonances occurring in the manifold junction and yield total reflection at some frequencies

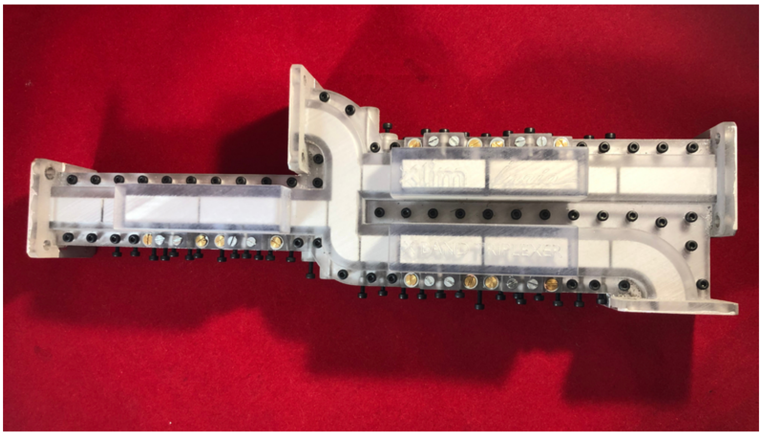


Figure 8. Compact triplexer synthesized via matrix multi-point interpolation techniques and realized via 3D printing.

of the channel ports. When latter coincide with the matching frequencies of a particular channel filter, the simultaneous matching problem has no solution, and the continuation algorithm fails irredeemably.

We therefore gave a full characterization of this manifold peaks and designed a heuristic approach to avoid their appearance during the continuation process. We showed that they only depend on the out of band response of the channel filters, and can in first approximation be considered as constant along the continuation process and estimated by a full wave simulation of each channel filter. This is then used within a triangular adjustment procedure that looks for possible manifold length adjustments (within the channel filters, and between that channel filters and the manifold junction) that guaranties the absence of manifold peaks within the band of each channel filter. Details of this procedure that give important information to the designer about the feasibility of an effective multiplexer response by means of given manifold T-junction, and this before any channel filter optimization procedure, are detailed in [23], [18] and were presented at Eumc 2019. In connection with the previously described continuation procedure, it was used to design a compact triplexer, based on frequency specifications considered as «hard to fulfill» and furnished by CNES. The triplexer was then realized using 3D printing techniques at Xlim (S. Bila and O. Tantot) our long standing academical partners on these topics (see Figure 8). This work is part of the PhD thesis [14] defended by David Martinez Martinez at the end of June.

6.2.2. Uniform matching and global optimality considerations: application to a reference tracking problem

This problem was proposed by Pauline Kergus, PhD student at Onera (Toulouse). In her PhD, she studied the following data driven problem: given frequency measurements of a plant, find a controller which allows to follow a given reference model. The approach she proposed was to directly identify the controller from frequency measurements induced on the controller by the closed loop. Of course the quality of the controller, and in particular its stability, highly depend on the chosen reference model. The question is thus: how to choose a good reference model M with a minimum of information on the plant? The reference model is linked to the sensitivity function S by the relation $M + S = 1$. The sensitivity function is an important design tool in control. To ensure closed loop stability, it should be stable and satisfy some interpolation conditions at the unstable poles and zeros of the plant [28]. Its shape reflect the performances of the closed loop: S should be small at low frequencies to ensure a good tracking accuracy, as well as disturbance rejection; while to ensure noise rejection, S should go to 1 at infinity (the reference model $1 - S$ should be small at high frequencies). The shaping problem for the sensitivity function can be stated in a manner almost similar to the matching problem described below: find a Schur function with minimum infinite norm in a frequency band $[0, w_c]$, where w_c is the chosen cutoff frequency, while satisfying some interpolatory constraints. The main difference that prevents for using the convex relaxation method proposed below is the condition at infinity. An alternative optimization method is under study. To get a non-optimal solution to the problem, Pauline Kergus proposed a simple way to enforce the interpolation conditions from a given well-shaped reference model. To compute the unstable poles and zeros of the plant, which is the minimal required information, she uses our software PISA https://project.inria.fr/pisa/working/project/. Examples illustrating the advantages and limitations of the method were studied. The results were reported in the journal paper [17] and presented at the CDC 2019 in Nice.

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 and oscillators, in particular to detect instability at an early stage of the design. This topic is studied in the doctoral work of S. Fueyo, co-advised with J.-B. Pomet (from the McTao Inria project-team). Application to oscillator design methodologies is studied 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. For devices operating at relatively low frequencies, time domain simulations perform satisfactorily to check stability. 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 a simple electrical wire at low frequency) becomes so small that simulations are intractable in reasonable time. Moreover, most linear components of such circuits are known through their frequency response, and a preliminary, numerically unstable step is then needed to obtain their impulse response, prior to any time domain simulation.

For these reasons, the analysis of such systems is carried out 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 component can be studied *via* the transfer impedance functions computed at some ports of the circuit. In recent years, we showed that under realistic dissipativity assumptions at high frequency for the building blocks of the circuit, these transfer functions are meromorphic in the complex frequency variable s, with at most finitely many unstable poles in the right half-plane [4]. 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 [11], that was further improved in [10] to address the design of oscillators, in collaboration with Smain Amari. This has resulted in the development of a software library called Pisa (see Section 3.4.1 , aiming at making these techniques available to practitioners. Research in this direction now focuses on the links between the width of the measurement band, the density of the measurement points, and the precision with which an unstable pole, located within a certain depth into the complex plane, can be identified.

Extensions of the procedure to the strong signal case, where linearisation is considered around a periodic trajectory, have received attention over the last two years. When stability is studied around a periodic trajectory, 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 present setting which is infinite dimensional, due to the presence of delays. Dwelling on the theory of retarded systems, S. Fueyo's

PhD work has shown last year that, for general circuits, the monodromy operator of the linearized system along its periodic trajectory is a compact perturbation of a high frequency, non dynamical operator, which is stable under a realistic passivity assumption at high frequency. Therefore, only finitely many unstable points can arise in the spectrum of the monodromy operator, and this year we established a connection between these and the singularities of the harmonic transfer function, viewed as a holomorphic function with values in periodic L^2 functions. One difficulty, however, is that these singularities need not affect all Fourier coefficients, whereas harmonic balance techniques can only estimate finitely many of them. This issue, that was apparently not singled out by practitioners, is currently under examination.

We also wrote an article reporting about the stability of the high frequency system, and recast this result in terms of exponential stability of certain delay systems [24].

6.4. The Hardy-Hodge decomposition

Participants: Laurent Baratchart, Masimba Nemaire.

In a joint work with T. Qian and P. Dang from the university of Macao, we proved in previous years that on a 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, provided that $2-\varepsilon<p<2+\varepsilon'$, 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 holds on Lipschitz surfaces (not just hypersurfaces), The Hardy-Hodge decomposition generalizes the classical Plemelj formulas from complex analysis. We pursued this year the writing of an article on this topic, and we also found that this decomposition yields a description of silent magnetizations distributions of L^p-class on a surface. A natural endeavor is now to use this description, *via* balayage, to describe volumetric silent magnetizations.

6.5. Identification of resonating frequencies of compact metallic objects in electromagnetic inverse scattering

Participants: Laurent Baratchart, Martine Olivi, Fabien Seyfert.

We started an academic collaboration with LEAT (Univ. Nice, France, pers. involved: Jean-Yves Dauvignac, Nicolas Fortino, Yasmina Zaki) on the topic of inverse scattering using frequency dependent measurements. As opposed to classical electromagnetic imaging where several spatially located sensors are used to identify the shape of an object by means of scattering data at a single frequency, a discrimination process between different metallic objects is here being sought for by means of a single, or a reduced number of sensors that operate on a whole frequency band. For short the spatial multiplicity and complexity of antenna sensors is here traded against a simpler architecture performing a frequency sweep.

The setting is shown on Figure 9 . The total field $E_t(r,\theta,\phi)$ is the sum of the incident field E_i (here a plane wave) and scattered field E_s, that is at every point in space we have $E_t=E_i+E_s$. A harmonic time dependency ($e^{j\omega t}$, where j is the imaginary unit: $j^2=-1$) is supposed for the incident wave, so that by linearity of Maxwell equations and after a transient state, following holds,

$$E_s(r_o,\theta_o,\phi_o)=H(s=j\omega,\theta_o,\phi_o)E_i(r_e,\theta_e,\phi_e).$$

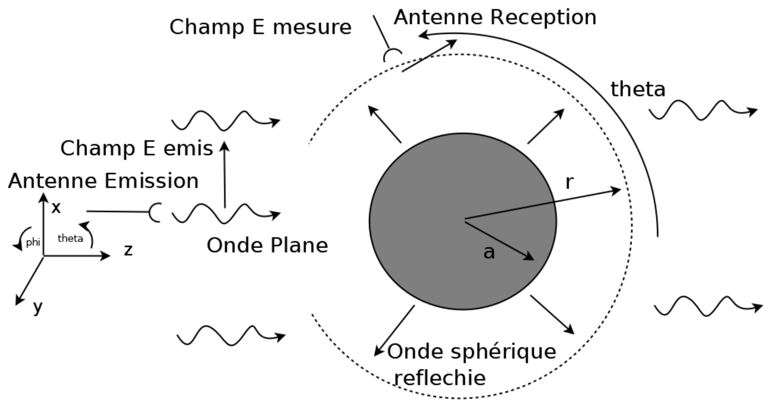


Figure 9. Sphere illuminated by an electromagnetic plane wave - measurement of the scattered wave

The subscripts o and e stand here for «observation point» and «emission point»: the scattered field at the observation point is therefore related to the emitted planar wave field at the emission point via the transfer function $H(s = j\omega, \theta_o, \phi_o)$. The emission point is here supposed fixed, so the dependency in e is omitted in H. Under regularity conditions on the scatterer's boundary the function H can be shown to admit an analytic continuation into the complex left half plane for the s variable, away from a discrete set (with a possible accumulation point a infinity) where it admits poles. Thus, H is a meromorphic function in the variable s. Its poles are called the resonating frequencies of the scattering object. Recovering these resonating frequencies from frequency scattering measurement, that is measurements of H at particular $s = j\omega_i's$ is the primary objective of this project.

In order to gain some insight we started a full study of the particular case when the scatterer is a spherical PEC (Perfectly Electric Conductor). In this case Maxwell equations can be solved «explicitly» by means of expansions in series of vectorial spherical harmonics. We showed in particular that in this case H admits following simple structure:

$$H(\omega, \theta_o, \phi_o) = R(s, \theta_o, \phi_o)e^{-\tau_1(\theta_o,\phi_o)s} + C(\theta_o, \phi_o)e^{-\tau_2(\theta_o,\phi_o)s},$$

where R is a meromorphic functions with poles at zeros of the spherical Hankel functions and their derivatives and C is independent of the frequency. Identification procedures, surprisingly close to the ones we developed in connection with amplifier stability analysis, are currently being studied to gain information about the resonating frequencies by means of a rational approximation of the function R once it has been de-embedded. Generalization of this analysis and procedure will be considered for arbitrarily compact PEC objects.

6.6. Imaging and modeling ancient materials

Participants: Vanna Lisa Coli, Juliette Leblond, Pat Vatiwutipong.

This is a recent activity of the team, linked to image classification in archaeology in the framework of the project ToMaT (see Regional Initiatives below) 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 images 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 in binary 3-D images, to which we apply a process named Hough transform (derived from Radon transform). This method, of which the generalization from 2-D to 3-D is quite recent, allows us to evaluate the presence of parallel lines going through the pores. The quantity of such lines is a good indicator of the “coiling” manufacturing, that it allows to distinguish from the other “spiral patchwork” patchwork technique, in particular. These progresses are described in [20], [22], [21], and the object of an article in preparation.

The Hough and Radon transforms can also be applied to 2-D slices of the available 3-D images displaying pores locations. In this framework, the use of Radon transform to evaluate the density of points in the image that do belong to (or almost) parallel lines appears to be quite efficient, as was seen during P. Vatiwutipong’s internship.

Other possibilities of investigation will be analyzed as well, such as machine learning techniques.

6.7. Behavior of poles in rational and meromorphic approximation

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Martine Olivi, Fabien Seyfert.

6.7.1. Rational approximation

The numerous experiments that we performed on synthetic data in the context of the MagLune project (see Sections 6.1.2 and 8.2.1) revealed an intriguing behavior of the local minima of the optimization problem underlying our method. In the context of that application, we are provided with sampled values on the unit circle $\mathbb{T}$ of a function f which is known to be of the form $f(z) = p(z)/(z-\beta)^5$ where $p(z) \in \mathbb{C}_4[z]$ is a polynomial of degree at most 4 with complex coefficients and $\beta \in \mathbb{D}$ belongs to the unit disk. A key problem consists in recovering β from the values of f on the unit circle. The same problem occurs in the core of FindSources3D (see 3.4.3 and 6.1.3) with p being of degree at most 2 and a pole of order 3 rather than 5.

In order to estimate β, we seek for the global minimum on $\mathbb{C}_4[z] \times \mathbb{D}$ of the function ϕ defined by

$$\phi : (q,\, \alpha) \mapsto \left\| \frac{q(z)}{(z-\alpha)^5} - f(z) \right\|_{L^2(\mathbb{T})}.$$

When f is actually a rational function of the considered form, ϕ obviously has a unique global minimum where it reaches the value 0. We experimentally observed that ϕ usually has several local minima, some of them achieving very small values, and these minima often have a complex argument close to the argument of β. This behavior is unusual and contrasts with the fact the function

$$\psi : (q, \alpha_1, \cdots, \alpha_5) \mapsto \left\| \frac{q(z)}{\prod_{i=1}^{5}(z-\alpha_i)} - f(z) \right\|_{L^2(\mathbb{T})}$$

is known to have a unique local minimum on $\mathbb{C}_4[z] \times \mathbb{D}^5$ (which is global) when f is a rational function of the same form.

In order to understand the reasons underlying our observations, we started studying the theoretical properties of the critical points of ϕ, in the general case of a pole of order $n \in \mathbb{N}^*$ and with a polynomial of degree less or equal to $n-1$ at the numerator. Our results so far are the following.

We introduce the family $(g_j^{(\alpha)})_{j\in\mathbb{N}^*}$ where $g_j^{(\alpha)}(z) = (1-\overline{\alpha}z)^{j-1}/(z-\alpha)^j$ which is an orthogonal basis (for the usual $L^2(\mathbb{T})$ Hilbert product) of the space of rational functions with a single pole (of arbitrary order) in α. Thanks to this family, we prove that (q,α) is a critical point of ϕ if and only if f is orthogonal either to $g_n^{(\alpha)}$ or $g_{n+1}^{(\alpha)}$ and, for such a given α, $q/(z-\alpha)^n$ is the orthogonal projection of f onto the rational functions of that form. The case when f is orthogonal to $g_n^{(\alpha)}$ combined with the fact that $q/(z-\alpha)^n$ is the orthogonal projection of f implies a pole-zero simplification of $q/(z-\alpha)^n$ at $z=\alpha$ and we conjecture that it exactly corresponds to local *maxima* of ϕ with respect to variable α. We also conjecture that the other case exactly corresponds to local *minima* of ϕ. We are currently working on proving these conjectures, which should not be too hard.

We also obtained an explicit algebraic equation characterizing α, and we know how to solve it when f is of the form $1/(z-\beta)^k$ ($1 \le k \le n$). For small values of n, we proved (and conjecture that it holds for any n) that there are $2k-1$ solutions in the unit disk, all lying on the diameter passing though β. This is a remarkable result that somehow theoretically confirms the kind of experimental observations we got. The theoretical case of a function f with a non trivial numerator seems currently out of reach, though.

6.7.2. Meromorphic approximation

We showed that best meromorphic approximation on a contour, in the uniform norm, to functions with countably many branched singularities with polar closure inside the contour produces poles whose counting measure accumulate weak-* to the Green equilibrium distribution on the cut of minimal capacity outside of which the function is single-valued. This is joint work with M. Yattselev (University of Indianapolis, Purdue University at Indianapolis). An article is currently being written on this topic.

I4S Project-Team

6. New Results

6.1. System identification

6.1.1. On Local LTI Model Coherence for LPV Interpolation

Participant: Qinghua Zhang.

In the local approach to linear parameter varying (LPV) system identification, it is widely acknowledged that locally estimated linear state-space models should be made coherent before being interpolated, but the accurate meaning of the term " coherent " or " coherence " is rarely defined. The purpose of this study is to analyze the relevance of two existing definitions and to point out the consequence of this analysis on the practice of LPV system identification. This work has been carried out in collaboration with Lennart Ljung of Linköping University and Rik Pintelon of Vriije Universiteit Brussel, and the results have been published in [22].

6.1.2. Stability Analysis of the Kalman Predictor

Participant: Qinghua Zhang.

The stability of the Kalman filter, though less often mentioned than the optimality in the recent literature, is a crucial property for real time applications. The purpose of this paper is to complete the classical stability analysis of the Kalman filter for general time varying systems. A proof of the stability of the one step ahead predictor, which is embedded in the Kalman filter, is presented in this paper, whereas the classical results were focused on the stability of the filter. The predictor stability is particularly important for linear parameter varying (LPV) system identification by means of prediction error minimization. This work has been carried out in collaboration with Liangquan Zhang of Beijing University of Posts and Telecommunications, and the results have been published in [23].

6.1.3. Regularized Adaptive Observer to Address Deficient Excitation

Participant: Qinghua Zhang.

Adaptive observers are recursive algorithms for joint estimation of both state variables and unknown parameters. Usually some persistent excitation (PE) condition is required for the convergence of adaptive observers. However, in practice, it may happen that the PE condition is not satisfied, because the available sensor signals do not contain sufficient information for the considered recursive estimation problem, which is ill-posed. To remedy the lack of PE condition, inspired by typical methods for solving ill-posed inverse problems, this paper proposes a regularized adaptive observer for general linear time varying (LTV) systems. Regularization terms are introduced in both state and parameter estimation recursions, in order to preserve the state-parameter decoupling transformation involved in the design of the adaptive observer. Like in typical ill-posed inverse problems, regularization implies an estimation bias, which can be reduced by using prior knowledge about the unknown parameters. This work has been carried out in collaboration with Fouad Giri and Tarek Ahmed-Ali of Université de Normandie, and the results have been presented at [40].

6.2. Damage detection and localization

6.2.1. Model sensitivity clustering for damage localization

Participants: Michael Doehler, Laurent Mevel.

The purpose of this paper is the development of a working damage localization method that is applicable on real data from complex structures. To achieve this goal, robust hypothesis tests are used, the sensitivity computation of the previously published residual is revisited for more precision thanks to reduced modal truncation errors, and an adequate clustering approach is proposed for the case of a high-dimensional FE parameterization for complex structures. Finally, an application of this framework is shown for the first time on experimental data for damage localization, namely in an ambient vibration test of a 3D steel frame at the University of British Columbia. [16]

6.2.2. Robustness to temperature changes for damage localization

Participants: Laurent Mevel, Michael Doehler, Alexander Mendler.

For structures in operation, temperature has been shown to be a major nuisance to the efficiency of such methods since the modal parameters are varying not only with damage but also due to temperature variations. For detection, environmental variation is hardly taken into account in localization approaches. In this paper, we propose a sensitivity-based correction of the identified modal parameters in the damaged state with respect to the temperature field in the reference state, based on a sensitivity analysis with respect to temperature dependent parameters of the finite element model in the reference state. The approach is then applied to the Stochastic Dynamic Damage Locating Vector (SDDLV) method, where its improved performance under non-uniform temperature variations is shown in a numerical application on a beam. [18], [26]

6.2.3. Robustness to temperature changes for damage detection

Participants: Laurent Mevel, Michael Doehler, Qinghua Zhang, Eva Viefhues.

Temperature affected vibration data is evaluated with a stochastic damage detection method, which relies on a null space based residual. A new approach is proposed, using model interpolation, where a global reference model is obtained from data in the reference state at several reference temperatures. Then, for a particular testing temperature, a local reference model is derived from the global reference model. Thus, a well fitting reference null space for the formulation of the residual is available when new data is tested for damage at arbitrary temperatures. Particular attention is paid to the computation of the residual's covariance, taking into account the uncertainty related to the null space estimate. This improves the test performance, resulting in a high probability of detection (PoD) of the new interpolation approach for global and local damages compared to previous approaches. [37]

6.3. Infrared Thermography

6.3.1. Long term thermal monitoring by standard passive Infrared thermography

Participants: Thibaud Toullier, Jean Dumoulin, Laurent Mevel.

The framework of latest technological improvements in low-cost infrared cameras have brought new opportunities for long-term infrastructures monitoring. Anyway, the accurate measurement of surfaces temperatures is facing the lack of knowledge of radiatives properties of the scene. By using multi-sensors instrumentation, the measurement model can be refined to get a better estimate of the temperature. To overcome a lack of sensors instrumentation, it has been shown that online and free available climatic data can be used. [15].

6.3.2. Long term thermal monitoring by multi-spectral infrared thermography

Participants: Thibaud Toullier, Jean Dumoulin, Laurent Mevel.

Bayesian methods to estimate simultaneously the emissivity and temperature have been developed and compared to literature's methods. A radiative exchange simulator of 3D scenes have been developed to compare those different methods on numerical data. This new software uses the hardware acceleration as well as a GPGPU approach to reduce the computation time. As a consequence, obtained numerical results emphasized an advanced use of multi-spectral infrared thermography for the monitoring of structures. This simultaneous estimation enables to have an estimate of the temperature by infrared thermography with a known uncertainty. [15].

6.4. Sensor and hardware based research

6.4.1. Fiber optic and interferometry

Participants: Xavier Chapeleau, Antoine Bassil.

The assessment of Coda Wave Interferometry (CWI) and Distributed Fiber Optics Sensing (DFOS) techniques for the detection of damages in a laboratory size reinforced concrete beam is presented in this paper. The sensitivity of these two novel techniques to micro cracks is discussed and compared to standard traditional sensors. Moreover, the capacity of a DFOS technique to localize cracks and quantify crack openings is also assessed. The results show that the implementation of CWI and DFOS techniques allow the detection of early subtle changes in reinforced concrete structures until crack formation. With their ability to quantify the crack opening, following early detection and localization, DFOS techniques can achieve more effective monitoring of reinforced concrete structures. Contrary to discrete sensors, CWI and DFOS techniques cover larger areas and thus provide more efficient infrastructures asset management and maintenance operations throughout the lifetime of the structure.

6.4.2. Offset Tracking of sensor clock using Kalman filter for wireless network synchronization

Participants: David Pallier, Vincent Le Cam, Qinghua Zhang.

Wireless Sensors Networks (WSN) are more and more used in structural health monitoring applications since they represent a less expensive and non-invasive way to monitor infrastructures. Most of these applications work by merging or comparing data from several sensors located across the structure. These data often comprise measurements of physicals phenomenons evolving with time, such as acceleration and temperature. To merge or compare time-dependent data from different sensors they need to be synchronized so all the samples are time-stamped with the same time reference. An initial synchronization of the sensors is needed because sensors are independent and therefore can not be all started at the same time. Subsequent re-synchronizations are also needed since the sensors keep track of time using their imperfect local clock. This work has been presented in [34].

6.4.3. Wireless implementation of system identification techniques

Participants: Michael Doehler, Mathieu Le Pen, Vincent Le Cam, Laurent Mevel.

Embedded wireless platforms such as the PEGASE platform are appealing and suitable to collect vibration data and then perform off-line and remote computation easily. To obtain detailed modal information of large and very large structures, many sensors would be required to cover the geometry of the structure with a reasonable accuracy. However, when only a limited amount of sensors is available, large structures can be measured in several sensor setups, where some sensors remain fixed and some are moved between different measurement setups. With the sensors connected to different wireless platforms, the synchronous acquisition of data is required. In this paper, a solution of data acquisition synchronization, as well as signal processing for merging the information taking into account the change of sensor positions and environmental variability is presented.

6.4.4. Management of Cloud architectures

Participants: Jean Dumoulin, Laurent Mevel.

Cloud2IR is an autonomous software architecture, allowing multi-sensor connection, dedicated to the long term thermal monitoring of infrastructures. The system has been developed in order to cut down software integration time facilitating the system adaptation to each experiment. First, a generic unit, a data management side able to aggregate any sensor data, type or size, automatically encapsulating them in various generic data format such as hierarchical data format or cloud data such as opengis standard. This whole part is also in charge of the acquisition scenario, the local storage management and the network management. Second, a specialized unit where the sensor specific development fitted to experimental requirements are addressed. The system has been deployed on two test sites for more than one year. It aggregates various sensor data issued from infrared thermal cameras, GPS units, pyranometers, weather stations. The software and some results in outdoor conditions are discussed

MCTAO Project-Team

7. New Results

7.1. Analysis of singularities in minimum time control problems

Participants: Jean-Baptiste Caillau, Jacques Féjoz [Université Paris-Dauphine & Observatoire de Paris], Michaël Orieux [SISSA], Robert Roussarie [Université de Bourgogne-Franche Comté].

An important class of problems is affine control problems with control on the disk (or the Euclidean ball, in higher dimensions). Such problems show up for instance in space mechanics and have been quite extensively studied from the mathematical (geometric) and numerical point of view. Still, even for the simplest cost, namely time minimization, the analysis of singularities occuring was more or less open. Building on previous results of the team and on recent studies of Agrachev and his collaborators, we give a detailed account of the behaviour of minimum time extremals crossing the so-called singular locus (typically a switching surface). The result is twofold. First, we show that there the set of initial conditions of the Hamiltonian flow can be stratified, and that the flow is smooth on each stratum, one of them being the codimension stratum leading to the singular locus. This generalizes in higher codimension the known case of switching conditions of codimension one encountered, for instance, in L^1-minimization (consumption minimization, in aerospace applications). We give a clear geometric interpretation of this first result in terms of normally hyperbolic invariant manifold. Secondly, we provide a model for the singularity on the flow when strata are crossed, proving that it is of logarithmic type. This paves the way for *ad hoc* numerical methods to treat this kind of extremal flow. The crucial tool for the analysis is a combination of blow-up and normal form techniques for dynamical systems.

7.2. The Sard Conjecture in sub-Riemannian Geometry

Participants: Ludovic Rifford, André Belotto Da Silva [Univ. Aix-Marseille], Adam Parusinski [Univ. Côte d'Azur].

In a work in progress, we address the Sard conjecture for sub-Riemannian structures on analytic manifolds and related problems. We present a description of singular horizontal curves of a totally nonholonomic analytic distribution in term of the projections of the orbits of some integrable and isotropic subanalytic distribution in the cotangent bundle. In the generic smooth case, we obtain a extension of an important result by Chitour, Jean and Trélat by showing that singular curves are the projection of a Hamiltonian singular vector field. As a by-product of our first result, we obtain a proof of the so-called minimal rank Sard conjecture in some analytic cases. It establishes that from a given point the set of points accessible through singular horizontal curves of minimal rank, which corresponds to the rank of the distribution, has Lebesgue measure zero under additional technical assumptions.

7.3. Local controllability of magnetic micro-swimmers and more general classes of control systems

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

As a part of Clément Moreau's PhD, we gave fine results on local controlability of magnetized micro swimmers actuated by an external magnetic field. We had shown that the "two-link" magnetic swimmer had some local controllability around its straight configuration but that it was not Small Time Locally Controllable" (STLC) in the classical sense that asks that poin ts close to the initial condition can be reached using "small" controls.

We derived in [30] some necessary conditions for STLC of affine control systems with two scalar controls, around an equlibrium where not only the drift vector field vanishes but one of the two control vector fields vanishes too; we state various necessary conditions (involving the value at the equilibrium of some iterated Lie brackets of the system vector fields), where the "smallness" of the controls is intended in the L^∞ (classical) or $W^{1,\infty}$ (less classical, used in recent work by K. Beauchard and F. Marbach).

We also arrived to local controllability results in higher dimension than the “two-link” micro-robots, see [9]. This relies on the following remark: classical STLC does not hold, but STLC is concerned with small controls, hence with variations around the zero control... but, due to one of the control fields vanishing, the system also rests at the equilibrium for (infinitely many) nozero constant values of the control. It is proved that there is one nonzero value of the control such that STLC holds when considered *around this constant control* and not around the zero control. In other terms, classical STLC holds after a constant feedback transformation.

7.4. Time-optimal deorbiting maneuvers of solar sails

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

Increasing interest in optimal low-thrust orbital transfers was triggered in the last decade by technological progress in electric propulsion and by the ambition of efficiently leveraging on orbital perturbations to enhance the maneuverability of small satellites. This work was aimed at investigating time optimal propellantless deorbiting maneuvers in low-Earth orbit using solar sails. The solution of this problem was achieved by doubly averaging the optimal control Hamiltonian with respect to both satellite and Sun longitudes. Initial conditions for the osculating trajectory were inferred via a near-identity transformation that approximates the quasi-periodic oscillations of both state and adjoint variables [61]. The outcomes of the study were presented at the 4th KePASSA meeting in Logrono [18].

7.5. Long-term evolution of quasi-satellite orbits

Participants: Lamberto Dell’Elce, Nicola Baresi [Univ. of Surrey, UK], Josué Cardoso Dos Santos [Sao Paulo State Univ., Brazil], 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, started in 2018 in collaboration with JAXA, investigates the navigability of mid- and high-altitude QSOs in terms of relative orbit element. Our developments are based on the Yamanaka-Ankersen solution of the Tschauner-Hempel equations and capture the effects of the secondary’s gravity and orbital eccentricity on the shape and orientation of near-equatorial retrograde relative orbits. The analytic solution that we obtained by averaging the equations of motion with respect to the longitude of the satellite is suitable to gain insight into the long-term evolution of QSOs. These results were recently published in [38].

7.6. Non-singular analytical solution of perturbed satellite motion using Milankovitch elements

Participants: Lamberto Dell’Elce, Pini Gurfil [Technion, Israel], Gianpaolo Izzo [Technion, Israel], Aaron J. Rosengren [Univ. of Arizona, US].

In the brief span of time after the launch of Sputnik, a whole succession of analyses was devoted to the problem poised by the drag-free motion of an artificial satellite about an oblate planet, employing almost every known perturbation method. Although in a sense, the problem is a classic one that also occurred among the natural satellites, it was necessary in the applications of artificial satellite motion to obtain a more general, detailed, and accurate solution. In this study, we developed a new formulation of the mean-to-osculating conversion for first-order oblateness perturbations based on the Milankovitch elements [74] that corrects the critical-inclination deficiency. We use the direct method of Kozai [67], and present an explicit analytical short-period correction in vector form that is valid for all orbits with nonzero angular momentum. Preliminary results were presented at the International Symposium of Space Flight Mechanics (ISSFM) [19].

7.7. Sub-Riemannian Geometry and Micro-Swimmers and Extensions to Control in Hydrodynamics

Participants: Bernard Bonnard, Piernicola Bettiol [Univ. Bretagne Ouest], Alice Nolot [Univ. de Bourgogne Franche Conté], Jérémy Rouot.

We pursue our study concerning the 1-copepod swimmer using techniques from SR-geometry and numerical simulations, see [40] for previously obtained results. Following Takagi model, a 2d-swimmer is currently analyzed whose aim is to perform a 2d-motion where the copepod swimmer can change its orientation. Preliminary study concerning this problem was analysed during the internship of A. Lenc in relation with the motion planning of a car. Under the impulse of O. Cots and B. Wembe an extension of the project is the developments of the geometric optimal control techniques in hydrodynamics. In particular we studied a Zermelo navigation problem in a current with a vortex [25] (submitted to ESAIM-COCV). An interesting and new phenomenon detected in optimal control is the existence for the geodesic flow of a Reeb foliation.

7.8. Swimming at low Reynolds number an optimal control problem

Participants: François Alouges [École Polytechnique], Luca Berti, Antonio Desimone [SISSA Trieste], Yacine El Alaoui-Faris, Laetitia Giraldi, Yizhar Or [Technion, Israel], Christophe Prud'Homme [Univ. de Strasbourg], Jean-Baptiste Pomet, Stéphane Régnier [Sorbonne Université], Oren Wiezel [Technion, Israel].

This part is devoted to study the displacement of micro-swimmers. We attack this problem using numerical tools and optimal control theory. Micro-scale swimmers move in the realm of negligible inertia, dominated by viscous drag forces, the fluid is governed by the Stokes equation. We study two types of models. First, deriving from the PDE system, in [5] we use Feel++, a finite elements library in order to simulate the motion of a one-hinged swimmer, which obeys to the scallop theorem. Then, we adress the flagellar microswimmers. In [31] we formulate the leading order dynamics of a $2D$ slender multi-link microswimmer assuming small-amplitude undulations about its straight configuration. The energy optimal stroke to achieve a given prescribed displacement in a given time period is obtained as the largest eigenvalue solution of a constrained optimal control problem. We prove that the optimal stroke is an ellipse lying within a two-dimensional plane in the $(N-1)$ dimensional space of shape variables, where N can be arbitrarily large. If the number of shape variables is small, we can consider the same problem when the prescribed displacement in one time period is large, and not attainable with small variations of the joint angles. The fully non-linear optimal control problem is solved numerically for the cases $N=3$ 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. Finally, in [28] we present an automated procedure for the design of optimal actuation for flagellar magnetic microswimmers based on numerical optimization. Using this method, a new magnetic actuation method is provided which allows these devices to swim significantly faster compared to the usual sinusoidal actuation. This leads to a novel swimming strategy which shows that a faster propulsion is obtained when the swimmer is allowed to go out-of-plane. This approach is experimentally validated on a scaled-up flexible swimmer.

7.9. Periodic body deformations are optimal for locomotion

Participants: Laetitia Giraldi, Frédéric Jean.

A periodic cycle of body's deformation is a common strategy for locomotion (see for instance birds, fishes, humans). The aim of this work (see [29]) is to establish that the auto-propulsion of deformable object is optimally achieved using periodic strategies of body's deformations. This property is proved for a simple model using optimal control theory framework.

7.10. Optimal Control of Chemical Networks by Temperature Control

Participants: Bernard Bonnard, Jérémy Rouot.

The objective of the project is to develop previous results obtained at the end of the 90's by B. Bonnard and his collaborators to control the production of batch reactors by temperature control in relation with the Shell Company. These results were derived to analyze the simple (but relevant for applications) irreversible reaction scheme $\mathrm{A} \to \mathrm{B} \to \mathrm{C}$. More complicated weakly reversible scheme like the McKeithan network are currently under investigation taking into account the bridge phenomenon detected in [7], where complicated optimal policies with two singular arcs can occur. Preliminary results are presented in [3] where also the geometric techniques are described. See also the article in the 58th IEEE-CDC Nice conference [11].

7.11. Muscular Isometric Force Contraction by Electric Stimulation

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

This project started two years ago under the impulse of T. Bakir (ImVia-UBFC) who defended his HDR on the subject (November, 2018). The problem is the one of optimizing the train pulses of the FES signal to produce the muscular contraction. It is based on the Hill model refined by Ding et al to take into account the variations of the fatigue variable. Preliminary closed loop results were obtained using an MPC-method where the state variable is estimated with an non linear observer [2]. The problem can be stated in the optimal sampled-control data framework; with the collaboration of L. Bourdin (Maths Dept Limoges), Pontryagin-type necessary conditions were derived and partially numerically implemented [1]. The project is supported by a PEPS 1 AMIES and a PGMO Project. A CIFRE Thesis is planned to start in January, 2020 (Phd Student: Quentin Arnaud) in the Company SEGULA, supervised by T. Bakir and co-Supervised by B. Bonnard. See section 8.1 .

7.12. Selection of microalgae

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

We investigate a minimal-time control problem in a chemostat continuous photo-bioreactor model that describes the dynamics of two distinct microalgae populations. Our objective is to optimize the time of separation between two species of microalgae by controlling the dilution rate. We focus on Droop's model. Using Pontryagin's principle, we develop a dilution-based control strategy that steers the model trajectories to a suitable target in minimal time. Our study reveals that the optimal solution has a turpike property [14] [27]. A numerical optimal-synthesis, based on direct optimal control tools, is performed in [15] and it shows that the optimal solution is of type bang-singular.

7.13. Extensions of the Zermelo-Markov-Dubins problem in optimal control

Participants: Ahmed Dieng, Jean-Baptiste Caillau, Jean-Baptiste Pomet, Sofya Maslovskaya.

Motivated by a collaboration with CGG in 2018, we continued investigating minimum time problems for simplified kinematic models of a marine vessel towing some equipments, with various curvature constraints. These are extensions (by adding the towed equipment) of the so-called Zermelo-Markov-Dubins problem. In [12], we describe the problem with the simplest possible model of the trailer, and show that the Hamiltonian system resulting from Pontryagin Principle for minimum time is integrable in that case, both for the "regular" flow and for the flow giving singular extremals; without giving an explicit analytic soltuon, this drastically simplifies the computation of optimal solutions; a description of the marine application solution is also given.

Ahmed Dieng's internship was the opportunity to test more complex models numerically and to have a qualitative approach of the results from [12].

Note that the collaboration with CGG (we had a short bilateral contract with this company in 2018) did not continue mainly because they stopped this activity and more generally marine acquisition. This recent press release details the transactions.

7.14. Stability of nonlinear high frequency amplifiers and stability of linear time-varying time-delay systems

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

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 non-linear stability analysis for periodic solutions and how it works with the results of harmonic identification. This is the topic of Sébastien Fueyo's PhD.

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. Publication in progress on this point, a preliminary version was presented in [17].

It was also the oppoprtunity to re-visit stibility of time-delay time-varying linear system. A new sufficient condition can be found in [22], and a more general result is the purpose of a publication to come. These result are important to the domain of linear time-delay systems because the time-varying case has sedom been touched.

NECS 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 [22] and in [48].

7.1.2. Boundary Control for Output Regulation in Scale-FreePositive Networks

Participants: D. Nikitin, C. Canudas-de-Wit [Contact person], P. Frasca.

This work addresses the problem of controlling aggregate quantities in large networks. More precisely, we deal with the problem of controlling a scalar output of a large-scale positive scale-free network to a constant reference value. We design an output-feedback controller such that no information about state vector or system matrices is needed. This controller can have arbitrary positivegains, and only one sufficient sign condition on system matricesshould be satisfied. This controller can be used to regulate the average state in a large-scale network with control applied to boundary nodes of the domain [51].

7.1.3. A functional approach to target controllability of networks

Participants: C. Commault, J. Van Der Woude [TU Delft], P. Frasca [Contact person].

In the control of networks, it is natural to consider the problem of controlling a limited number of *target nodes* of a network. Equivalently, we can see this problem as controlling the target variables of a structured system, where the state variables of the system are associated to the nodes of the network. We deal with this problem from a different point of view as compared to most recent literature. Indeed, instead of considering controllability in the Kalman sense, that is, as the ability to drive the target states to a desired value, we consider the stronger requirement of driving the target variables as time functions. The latter notion is called functional target controllability. We think that restricting the controllability requirement to a limited set of important variables justifies using a more accurate notion of controllability for these variables. Remarkably, the notion of functional controllability allows formulating very simple graphical conditions for target controllability in the spirit of the structural approach to controllability. The functional approach enables us, moreover, to determine the smallest set of steering nodes that need to be actuated to ensure target controllability, where these steering nodes are constrained to belong to a given set. We show that such a smallest set can be found in polynomial time. We are also able to classify the possible actuated variables in terms of their importance with respect to the functional target controllability problem. This research is reported in [16].

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

Participants: F. Garin [Contact person], A. Kibangou, S. Gracy [KTH Stockholm], S.m. Fosson [Politecnico di Torino].

Cyber-physical systems are composed of many simple components (agents) with interconnections giving rise to a global complex behaviour. One line or research on security of cyber-physical systems models an attack as an unknown input being maliciously injected in the system. 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: structural results, true for almost all interaction weights, and strongly structural results, true for all non-zero interaction weights. Our results in 2019 concern structural and strongly structural ISO for time-varying systems [19], strongly structural ISO for time-invariant systems [46]. Moreover in [44] we study delay-L left-invertibility, where the input reconstruction is allowed to take L time steps instead of requiring immediate reconstruction in a single step. We obtain preliminary results for structural delay-L left-invertibility, which include a full characterization for the case where the input is scalar, and for the cases where L is one and two, while the general case remains an open problem. When the conditions for ISO are satisfied, one can run well-known algorithms in the same vein as a Kalman filter, in order to reconstruct the state and the unknown input from noisy measurements. In [43], we consider cases where the system is not ISO, and we exploit compressive sensing techniques in order to obtain nevertheless a unique reconstruction of the input, under the assumption that the input is highly sparse (e.g., when only one or few states are under attack, albeit the attack position is unknown).

7.1.5. Collaborative monitoring of network structural robustness

Participants: A. Kibangou [Contact person], T.m.d. Tran [Univ. of Danang].

Interacting systems can be naturally viewed as networks modelled by graphs, whose vertices represent the components of the system while edges stand for the interactions between these components. The efficiency of a network of a network can be evaluated through its functional robustness and structural robustness. The former usually stands for robustness against noise while the latter is related to the network performance despite changes in network topology (node or edge failure). Structural robustness has been an important topic in various domains: in distribution networks (e.g. power or water distribution networks), breakdowns can prevent service to customers; in communication networks, equipment failures may disrupt the network and block users from communicating; in contact networks, removing nodes (persons) by means of vaccination can prevent epidemic propagation. In [31] we have considered the critical threshold of a network and the effective graph resistance (Kirchhoff index) of a sub-graph characterizing the interconnection of sub-networks, that are partitioned from the given network as robustness metric. In which, the critical threshold depends only on the two first moments of the degree distribution while the Kirchhoff index can be computed with Laplacian eigenvalues. Therefore, we show how to estimate jointly the Laplacian eigenvalues and the two first moments of the degree distribution in a distributed way.

7.1.6. Estimation of the average state in large scale networks

Participants: A. Kibangou [Contact person], C. Canudas-de-Wit, U. Niazi, D. Deplano [Univ. Cagliari].

State estimation for monitoring large-scale systems requires tremendous amounts of computational and sensing resources, which is impractical in most applications. However, knowledge of some aggregated quantity of the state suffices in several applications. Processes over physical networks such as traffic, epidemic spread, and thermal control are examples of large-scale systems. Due to the diffusive nature of these systems, the average state is usually sufficient for monitoring purposes. For instance, estimating the average traffic density in some sector of a traffic network helps to monitor the congestion effectively. In the event of an epidemic, estimating the average proportion of infected people over several towns, which are interconnected through people commuting for work or other purposes, helps to devise the preventive measures for controlling the epidemic spread. For the temperature regulation of a building, the thermistors can only be placed either on the walls or the roof, therefore, estimating the average temperature of the interior of a large corridor is crucial. Other examples include the averaging systems such as opinion networks and wireless sensor networks where the average state is of paramount importance. In [40] we address observability and detectability of the average state of a network system when few gateway nodes are available. To reduce the complexity of the problem, the system is transformed to a lower dimensional state space by aggregation. The notions of average observability and average detectability are then defined, and the respective necessary and sufficient conditions are provided. In [25] we provide a computationally tractable necessary and sufficient condition for the existence of an average state observer for large-scale linear time-invariant (LTI) systems. Two design procedures, each with its own significance, are proposed. When the necessary and sufficient condition is not satisfied, a methodology is devised to obtain an optimal asymptotic estimate of the average state. In particular, the estimation problem is addressed by aggregating the unmeasured states of the original system and obtaining a projected system of reduced dimension. This approach reduces the complexity of the estimation task and yields an observer of dimension one. Moreover, it turns out that the dimension of the system also does not affect the upper bound on the estimation error.

7.1.7. Structure-based Clustering Algorithm for Model Reduction of Large-scale Network Systems

Participants: C. Canudas-de-Wit [Contact person], U. Niazi, J. Scherpen [Univ. Groningen], X. Cheng [Univ. Groningen].

In [41], A model reduction technique is presented that identifies and aggregates clusters in a large-scale network system and yields a reduced model with tractable dimension. The network clustering problem is translated to a graph reduction problem, which is formulated as a minimization of distance from lumpability. The problem is a non-convex, mixed-integer optimization problem and only depends on the graph structure of the system. We provide a heuristic algorithm to identify clusters that are not only suboptimal but are also connected, that is, each cluster forms a connected induced subgraph in the network system.

7.2. Control of multi-agent systems and opinion dynamics

7.2.1. Robust average consensus over unreliable networks

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

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 [11] provides a complete account of our results.

7.2.2. Message-passing computation of harmonic influence in social networks

Participants: W. S. Rossi [Univ. Groningen], 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 [29], we prove that the algorithm converges on general graphs.

7.2.3. Hybrid models of opinion dynamics

Participants: P. Frasca [Contact person], S. Tarbouriech [LAAS CNRS], L. Zaccarian [LAAS CNRS].

Hybrid dynamical systems are a promising framework to model social interactions. In this research line, we are beginning to use tools from the theory of hybrid systems to study opinion dynamics on networks with opinion-dependent connectivity. According to the hybrid framework, our dynamics are represented by the combination of continuous flow dynamics and discrete jump dynamics. The flow embodies the attractive forces between the agents and is defined by an ordinary differential equation whose right-hand side is a Laplacian, whereas the jumps describe the activation or deactivation of the pairwise interactions between agents. We first reformulate the classical Hegselmann–Krause model in this framework and then define a novel interaction model, which has the property of being scale-invariant. We study the stability and convergence properties of both models by a Lyapunov analysis, showing convergence and clusterization of opinions [18].

7.2.4. Stability of Metabolic Networks

Participants: F. Garin [Contact person], B. Piccoli [Rutgers Univ. Camden], N. Merrill [Rutgers Univ. Camden], Z. An [Rutgers Univ. Camden], S. Mc Quade [Rutgers Univ. Camden].

Quantitative Systems Pharmacology (QSP) aims to gain more information about a potential drug treatment on a human patient before the more expensive stages of development begin. QSP models allow us to perform insilico experiments on a simulated metabolic system that predicts the response ofperturbing a flux. The methodology named LIFE (Linear-in-Flux Expressions) was developed with the purpose of simulating and analyzing large metabolic systems. These systems can be associated to directed graphs: the edges represent the reaction rates (fluxes), and the vertices represent quantities of chemical compounds (metabolites). In [23], we study LIFE systems, addressing two main problems: 1. for fixed metabolite levels, find all fluxes for which the metabolite levels are an equilibrium, and 2. for fixed fluxes, find all metabolite levels which are equilibria for the system. We show how stability analysis from the fields of network flows, compartmental systems, control theory and Markov chains apply to LIFE systems.

7.3. Transportation networks and vehicular systems

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

Participants: S. Baldi [Univ. Delft], 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 [12] and of output-feedback [14], under the assumption that the topology of the interconnections has no circuits. Further investigation on relaxing this restrictive assumption is in progress. We also showed that agents need no leader to synchronise, even in presence of heterogeneity [13].

7.3.2. Stability of vehicle platoons with AVs

Participants: V. Giammarino [Univ. Delft], M. Lv [Univ. Delft], P. Frasca [Contact person], M.l. Delle Monache, S. Baldi [TU Delft].

A key notion to understand the impact of Autonomous Vehicles on traffic is the notion of *stability* of the vehicle collective motion. In this line of research, we have sought criteria to determine when stop-and-go waves form in platoons of human-driven vehicles, and when they can be dissipated by the presence of an autonomous vehicle. Our analysis takes the start from the observation that the standard notion of string/ring stability definition, which requires uniformity with respect to the number of vehicles in the platoon, is too demanding for a mixed traffic scenario. The setting under consideration is the following: the vehicles run along a ring road and the human-driven vehicles obey a combined follow-the-leader and optimal velocity model, while the autonomous vehicle obeys an appropriately designed model. The criteria are tested on a linearized version of the resulting platoon dynamics and simulation tests using nonlinear model are carried out [45].

7.3.3. Control and estimation using autonomous vehicles

Participants: R. Stern [Vanderbilt University], S. Cui [Temple University], M.l. Delle Monache [Contact person], T. Liard, Y. Chen [Vanderbilt University], R. Bhadani [University of Arizona], M. Bunting [University of Arizona], M. Churchill [UIUC], N. Hamilton [Vanderbilt University], R. Haulcy [Yale University], H. Pohlmann [Temple University], F. Wu [UC Berkeley], B. Piccoli [Rutgers University], B. Seibold [Temple University], J. Sprinkle [University of Arizona], D.b. Work [Vanderbilt University].

It is anticipated that in the near future, the penetration rate of vehicles with some autonomous capabilities will increase on roadways. In [30], we analyze the potential reduction of vehicular emissions caused by the whole traffic stream, when a small number of autonomous vehicles are designed to stabilize the traffic flow and dampen stop-and-go waves. To demonstrate this, vehicle velocity and acceleration data are collected form a series of field experiments that use a single autonomous-capable vehicle to dampen traffic waves on a circular ring road with 20 to 21 human-piloted vehicles. From the experimental data, vehicle emissions (hydrocarbons, carbon monoxide, carbon dioxide, and nitrogen oxides) are estimated using the MOVES emissions models. We find that vehicle emissions of the entire fleet may be reduced by between 15% (for carbon dioxide) and 73% (for nitrogen oxides) when stop-and-go waves are reduced or eleiminated by the dampening action of the autonomous vehicle in the flow of human drivers. This is possible if a small fraction (5%) of vehicles are autonomous and designed to actively dampen traffic waves. In [57], we look at the problem of traffic control in which an autonomous vehicle is used to regulate human piloted traffic to dissipate stop and go traffic waves. We investigate the controllability of well-known microscopic traffic flow models: i) the Bando model (also known as the optimal velocity model), ii) the follow-the-leader model and iii) a combined optimal velocity – follow the leader model. Based on the controllability results, we propose three control strategies for an autonomous vehicles to stabilize the human piloted traffic. After, we simulate the control effects on the microscopic models of human drivers in numerical experiments to quantify the potential benefits of the controllers. Based on the simulations, finally we conduct a field experiment with 22 human drivers and a fully autonomous-capable vehicle, to assess the feasibility of autonomous vehicle based traffic control on real human piloted traffic. We show that both in simulation and in the field test an autonomous vehicle is able to dampen waves generated by 22 cars, and that as a consequence, the total fuel consumption of all vehicles is reduced by up to 20%. In [17], we consider a partial differential equation – ordinary differential equation system to describe the dynamics of traffic with autonomous vehicles. In the model the bulk flow is represented by a scalar conservation law, while each autonomous vehicle is described by a car following model. The autonomous vehicles act as tracer vehicles in the flow and collect measurements along their trajectory to estimate the bulk flow. The main result is to prove theoretically and show numerically how to reconstruct the correct traffic density using only the measurements from the autonomous vehicles.

7.3.4. Two-dimensional traffic flow models

Participants: S. Mollier, M.l. Delle Monache, C. Canudas-de-Wit [Contact person], B. Seibold [Temple University].

In [24], we introduce a new traffic flow model for a dense urban area. We consider a two-dimensional conservation law in which the velocity magnitude is given by the fundamental diagram and the velocity direction is constructed following the network geometry. The model is validated using synthetic data from Aimsun and a reconstruction technique to recover the 2D density from the data of individual vehicles is proposed. In [50], [49], we introduce a two dimensional and multi-layer traffic model with a new planning and decision making method in large scale traffic networks for predicting how traffic evolves in special events, emergencies and changes in the city mobility demands. The proposed method is based on a 2-D aggregated traffic model for large scale traffic networks which describes traffic evolution as a fluid in two space dimensions extended with additional state density variables, each one associated to a particular layer describing vehicles evolving in different directions. The model is a 2D-PDE described by a system of conservation laws. For this specific case, the resulting PDE is not anymore hyperbolic as typically the LWR model but results in a hybrid hyperbolic-elliptic PDE depending on the density level. In this case, usual numerical schemes may be not valid and often lead to oscillation in the solution. Thus, we consider a high order numerical scheme to improve the numerical solution. Finally, the model is used to predict how the typical traffic evolution will be impacted in particular scenarios like special events or changes in demands.

7.3.5. High-fidelity vehicle trajectory data

Participants: F. Wu [UC Berkeley], R. Stern [Vanderbilt University], S. Cui [Temple University], M.l. Delle Monache [Contact person], R. Bhadani [University of Arizona], M. Bunting [University of Arizona], M. Churchill [UIUC], N. Hamilton [Vanderbilt University], R. Haulcy [Yale University], B. Piccoli [Rutgers University], J. Sprinkle [University of Arizona], D.b. Work [Vanderbilt University], B. Seibold [Temple University].

High fidelity-vehicle trajectory data is becoming increasingly important in traffic modeling, especially to capture dynamic features such as stop-and-go waves. In [34], we present data collected in a series of eight experiments on a circular track with human drivers. The data contains smooth flowing and stop-and-go traffic conditions. The vehicle trajectories are collected using a panoramic 360-degree camera, and fuel rate data is recorded via an on-board diagnostics scanner installed in each vehicle. The video data from the 360-degree camera is processed with an offline unsupervised algorithm to extract vehicle trajectories from experimental data. The trajectories are highly accurate, with a mean positional bias of less than 0.01 m and a standard deviation of 0.11 m. The velocities are also validated to be highly accurate with a bias of 0.02 m/s and standard deviation of 0.09 m/s.

7.3.6. Robust tracking control design for fluid traffic dynamics

Participants: L. Tumash, C. Canudas-de-Wit [contact person], M.l. Delle Monache.

In [53] we analyze the boundary control of the traffic system described by the LWR model with a triangular fundamental diagram and a space-dependent indomain unknown disturbance, which can be described as an inhomogeneous transport equation. The controller design strategy aims first at stabilizing the deviation from the desired time-dependent trajectory and then at minimizing the deviation in the sense of two possible space-norms.

7.3.7. Urban traffic control

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

In [20] we study near-optimal operation of traffic lights in an urban area, e.g., a town or a neighborhood. The goal is on-line optimization of traffic lights schedule in real time, so as to take into account variable traffic demands, with the objective of obtaining a better use of the road infrastructure. More precisely, we aim at maximizing total travel distance within the network, together with balancing densities across the network. The complexity of optimization over a large area is addressed both in the formulation of the optimization problem, with a suitable choice of the traffic model, and in a distributed solution, which not only parallelizes computations, but also respects the geometry of the town, i.e., it is suitable for an implementation in a smart infrastructure where each intersection can compute its optimal traffic lights by local computations combined with exchanges of information with neighbor intersections.

7.3.8. Modeling and control strategies for improving environmental sustainability of road transportation

Participants: B. Othman, G. de Nunzio [IFP Energies nouvelles], D. Di Domenico [IFP Energies nouvelles], C. Canudas-de-Wit [Contact person].

As road transportation energy use and environmental impact are globally rising at an alarming pace, authorities seek in research and technological advancement innovative solutions to increase road traffic sustainability. The unclear and partial correlation between road congestion and environmental impact is promoting new research directions in traffic management. We review the existing modeling approaches to accurately represent traffic behavior and the associated energy consumption and pollutant emissions [26]. The review then covers the transportation problems and control strategies that address directly environmental performance criteria, especially in urban networks. A discussion on the advantages of the different methods and on the future outlook for the eco-traffic management completes the proposed survey.

7.3.9. Data analysis for smart multi-modal transportation planning

Participants: A. Kibangou [Contact person], T. Moyo [Univ. of Johannesburg], W. Musakwa [Univ. of Johannesburg].

Modern cities have managed to balance the relationship between supply and demand of services through clear planning strategies which advocate smart solutions to the ever increasing demand for public tranportation services. The end goal is not to prohibit citizens to use their private cars, but to create an enabling smart system at a suitable scale which would lead to citizens not needing to own or drive a car. Having an efficiently and effectively run public transportation system is a crucial and indispensable factor for any developing city region. However as the provision of public transportation is a multifaceted process, with intertwining elements such as culture, politics,finance and shareholder interests, smart means of monitoring and mitigating the challenges faced in the provision of public transportation need to be developed continuously. The Gauteng city region is likewise faced with this challenge. With this region being the economic hub of South Africa, this has greatly affected the operation of the Gautrain system and the BRT systems within the region, as more and more people require a fast and reliable transportation means to move in and out the metropolitan cities. The study relied on a questionnaire-based survey that was administered to 60 respondents. The questionnaire had both closed and open-ended questions which were administered online through Google forms so as to obtain a good response rate from commuters who reside within the study area. The questions centred on identifying factors influencing the commuter's travelling patterns. Gautrain Management Agency reports and literature were also utilised to supplement infomation gleaned from the questionnaire. Besides the questionnaire, secondary data was collected from Twitter (tweets) concerning the Gaubus and Gautrain (between the period of August to November 2018). Posts from 380 users were analysed. This data was used to spatially identify POI of Gaubus users and also to identify the spatial relationship between land use activities, Gaubus routes, Gaubus stops, Gautrain stations and Guatrain routes. A neighboorhood analysis was run using a focal statistics based tool to map the spatial distribution of commuters of the Gaubus [56].

7.3.10. Location of turning ratio and flow sensors for flow reconstruction in large traffic networks

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

We examine the problem of minimizing the number of sensors needed to completely recover the vehicular flow in a steady state traffic network [28]. We consider two possible sensor technologies: one that allows the measurement of turning ratios at a given intersection and the other that directly measures the flow in a road. We formulate an optimization problem that finds the optimal location of both types of sensors, such that a minimum number is required. To solve this problem, we propose a method that relies on the structure of the underlying graph, which has a quasi-linear computational complexity, resulting in less computing time when compared to other works in the literature. We evaluate our results using dynamical traffic simulations in synthetic networks.

7.4. Multisensor data fusion for navigation

7.4.1. Heterogeneity and uncertainty in distributed estimation from relative measurements

Participants: C. Ravazzi [Politecnico Torino], N.k. Chan [Univ. Groningen], P. Frasca [Contact person].

This work, presented in [27], 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.

7.4.2. Cooperative localization and navigation: Theory, research, and practice

Participants: C. Gao [Naval Aviation University, China], G. Zhao [Naval Aviation University, China], H. Fourati [Contact person].

The idea of the book [58] comes as a response to the immense interest and strong activities in the field of cooperative localization and navigation during the past few years, both in theoretical and practical aspects. This book is targeted toward researchers, academics, engineers, and graduate students working in the field of sensor fusion, filtering, and signal processing for localization and navigation. This book, entitled Cooperative Localization and Navigation: Theory, Research and Practice, captures the latest results and techniques for cooperative navigation drawn from a broad array of disciplines. It is intended to provide the reader with a generic and comprehensive view of contemporary state estimation methodologies for localization and navigation, as well as the most recent researches and novel advances on cooperative localization and navigation task exploring the design of algorithms and architectures, benefits, and challenging aspects, as well as a potential broad array of disciplines, including wireless communication, in-door localization, robotics, and emergency rescue. These issues arise from the imperfection and diversity of cooperative sources, the contention and collision of communication channels, the selection and fusion of cooperative data, and the nature of the application environment. The issues that make cooperative-based navigational state estimation a challenging task, and which will be discussed through the different chapters of the book, are related to (1) the nature and model of sensors and cooperative sources (e.g., range-based sensor, angle-based sensor, inertialsensor, and vision sensor); (2) the communication medium and cooperative strategies; (3) the theoretical developments of state estimation and data fusion; and (4) the applicable platforms.

7.4.3. Data fusion from multi-inertial and magnetic sensors

- **Attitude estimation from multi-sensor observations**

  Participants: J. Wu [Hong Kong University of Science and Technology], Z. Zhou [University of Electronic Science and Technology of China], H. Fourati [Contact person], R. Li [University of Electronic Science and Technology of China], M. Liu [Hong Kong University of Science and Technology], A. Kibangou, A. Makni.

  Focusing on generalized sensor combinations, we deal with attitude estimation problem using a linear complementary filter [36]. The quaternion observation model is obtained via a gradient descent algorithm (GDA). An additive measurement model is then established according to derived results. The filter is named as the generalized complementary filter (GCF) where the observation model is simplified to its limit as a linear one that is quite different from previous-reported brute-force computation results. Moreover, we prove that representative derivative-based optimization algorithms are essentially equivalent to each other. Derivations are given to establish the state model based on the quaternion kinematic equation. The proposed algorithm is validated under several experimental conditions involving free-living environment, harsh external field disturbances and aerial flight test aided by robotic vision. Using the specially designed experimental devices, data acquisition and algorithm computations are performed to give comparisons on accuracy, robustness, time-consumption and etc. with representative methods. The results show that not only the proposed filter can give fast, accurate and stable estimates in terms of various sensor combinations, but it also produces robust attitude estimation in the presence of harsh situations e.g. irregular magnetic distortion. In other recent work, related to the attitude estimation, we add some corrections to update that version [35]. In [21], we propose the design of an attitude estimation algorithm for a rigid body subject to accelerated maneuvers. Unlike the current literature where the process model is usually driven by triaxial gyroscope measurements, we investigate a new formulation of the state-space model where the process model is given by triaxial accelerometer measurements. The observation model is given by triaxial gyroscope and magnetometer measurements. The proposed model is written as a descriptor system and takes the external acceleration sensed by the accelerometer into account. Based on this model, a Quaternion Descriptor Filter (QDF) is developed and its performance is evaluated through simulations and experimental tests in pedestrian navigation.

- **Convexity analysis of optimization framework of attitude determination**
  Participants: J. Wu [Hong Kong University of Science and Technology], Z. Zhou [University of Electronic Science and Technology of China], H. Fourati [Contact person], M. Liu [Hong Kong University of Science and Technology].

  In the past several years, there have been several representative attitude determination methods developed using derivative-based optimization algorithms. Optimization techniques e.g. gradient-descent algorithm (GDA), Gauss-Newton algorithm (GNA), LevenbergMarquadt algorithm (LMA) suffer from local optimum in real engineering practices. A brief discussion on the convexity of this problem was presented recently, stating that the problem is neither convex nor concave. In our work, we give analytic proofs on this problem. The results reveal that the target loss function is convex in the common practice of quaternion normalization, which leads to non-existence of local optimum.

- **Behaviors classification based distance measuring system for pedestrians via a foot-mounted multi-inertial sensors**
  Participants: Z. Zhou [University of Electronic Science and Technology of China], S. Mo [University of Electronic Science and Technology of China], J. Wu [Hong Kong University of Science and Technology], H. Fourati [Contact person].

  We developed 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 [37]. Conventional methods for step detection and step length estimation cannot adapt well to the general pedestrian applications since the parameters in these methods may vary for different persons and motions. In this paper, 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. Finally, real experiments are carried out to verify our proposed step detection method and step length model. The results show that the proposed method outperforms the existing representative methods and it exhibits the merits of accuracy and adaptability for different persons in real time and significantly improves the accuracy of distance measuring.

- **Human activities and postures recognition: from inertial measurements to quaternion-based approaches**
  Participants: M. Zmitri, H. Fourati [contact person], N. Vuillerme [AGEIS, UGA].

  We present two approaches to assess the effect of the number of inertial sensors and their location placements on recognition of human postures and activities [38]. Inertial and Magnetic Measurement Units (IMMUs)—which consist of a triad of three-axis accelerometer, three-axis gyroscope, and three-axis magnetometer sensors—are used in this work. Five IMMUs are initially used and attached to different body segments. Placements of up to three IMMUs are then considered: back, left foot, and left thigh. The subspace k-nearest neighbors (KNN) classifier is used to achieve the supervised learning process and the recognition task. In a first approach, we feed raw data from three-axis accelerometer and three-axis gyroscope into the classifier without any filtering or pre-processing, unlike what is usually reported in the state-of-the-art where statistical features were computed instead. Results show the efficiency of this method for the recognition of the studied activities and postures. With the proposed algorithm, more than 80% of the activities and postures are correctly classified using one IMMU, placed on the lower back, left thigh, or left foot location, and more than 90% when combining all three placements. In a second approach, we extract attitude, in term of quaternion, from IMMUs in order to more precisely achieve the recognition process. The obtained accuracy results are compared to those obtained when only raw data is exploited. Results show that the use of attitude significantly improves the performance of the classifier, especially for certain specific activities. In that case, it was further shown that using a smaller number of features, with quaternion, in the recognition process leads to a lower computation time and better accuracy.

- **Improving inertial velocity estimation through magnetic field gradient-based extended kalman filter**
  Participants: M. Zmitri, H. Fourati [contact person], C. Prieur [GIPSA-Lab, UGA].

  We focused on the velocity estimation problem of a rigid body and how to improve it with magnetoinertial sensors-based theory [55]. We provide a continuous-time model that describes the motion of the body and we augment it after by introducing a new magnetic field gradient equation instead of using its value directly as an input for the model, as done usually in the corresponding literature. We investigate the advantage of moving to higher order spatial derivatives of the magnetic field in the estimation of velocity. These derivatives are computed thanks to a determined arrangement of magnetometers array. Within this framework, a specific set configuration of Extended Kalman Filters (EKFs) is proposed to focus mainly on the estimation of velocity and attitude of the body, but includes also an estimation of the magnetic field and its gradient. Some simulations for a specific scenario are proposed to show the improvements that we bring to the velocity estimation.

QUANTIC Project-Team

6. New Results

6.1. Highly coherent spin states in carbon nanotubes coupled to cavity photons

Participants: Zaki Leghtas

Spins confined in quantum dots are considered as a promising platform for quantum information processing. While many advanced quantum operations have been demonstrated, experimental as well as theoretical efforts are now focusing on the development of scalable spin quantum bit architectures. One particularly promising method relies on the coupling of spin quantum bits to microwave cavity photons. This would enable the coupling of distant spins via the exchange of virtual photons for two qubit gate applications, which still remains to be demonstrated with spin qubits. Here, we use a circuit QED spin-photon interface to drive a single electronic spin in a carbon nanotube based double quantum dot using cavity photons. The microwave spectroscopy allows us to identify an electrically controlled spin transition with a decoherence rate which can be tuned to be as low as 250kHz. We show that this value is consistent with the expected hyperfine coupling in carbon nanotubes. These coherence properties, which can be attributed to the use of pristine carbon nanotubes stapled inside the cavity, should enable coherent spin-spin interaction via cavity photons and compare favourably to the ones recently demonstrated in Si-based circuit QED experiments. This experimental result is a collaboration between Zaki Leghtas (QUANTIC) and the group of Takis Kontos at ENS and was published in [13].

6.2. Escape of a Driven Quantum Josephson Circuit into Unconfined States

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

Josephson circuits have been ideal systems to study complex nonlinear dynamics that 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 work, we show that these drives lead to an instability that 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 nonlinearities 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 experimental work published in [17] demonstrates elements of the theory derived by [22].

6.3. Structural Instability of Driven Josephson Circuits Prevented by an Inductive Shunt

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

Superconducting circuits are a versatile platform to implement a multitude of Hamiltonians that 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 in situ control of couplings, which cannot be obtained by near-equilibrium Hamiltonians. However, as shown in this theoretical study, out-of-equilibrium systems are easily plagued by complex dynamics, leading to instabilities. The prediction and prevention of 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 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 theoretical result was published in [22] and analyzes the experiment [17].

6.4. Fast and virtually exact quantum gate generation in $U(n)$ via Iterative Lyapunov Methods

Participants: Pierre Rouchon

This work presents an iterative algorithm published in [20] and named RIGA for Reference Input Generation Algorithm. This algorithm constructs smooth control pulses for quantum gate preparations of closed quantum systems. It combines right translation invariance and Lyapunov trajectory tracking. It exhibits exponential convergence when the system is controllable. It can be seen as a closed-loop version of the widely used GRAPE algorithm. Two numerical case-studies borrowed from the recent literature are addressed. The first one is relative to a system of 10 coupled qubits with local controls. The second one considers a C-NOT gate generation involving the lower levels of two coupled nonlinear cavities (transmon-qubits).

6.5. Benchmarking maximum-likelihood state estimation with an entangled two-cavity state

Participants: Pierre Rouchon

The efficient quantum state reconstruction algorithm described in the PhD of Pierre Six, a former student of the Quantic team, (see [89]) is experimentally implemented on the non-local state of two microwave cavities entangled by a circular Rydberg atom. In [19], we use information provided by long sequences of measurements performed by resonant and dispersive probe atoms over time scales involving the system decoherence. Moreover, we benefit from the consolidation, in the same reconstruction, of different measurement protocols providing complementary information. Finally, we obtain realistic error bars for the matrix elements of the reconstructed density operator. These results demonstrate the pertinence and precision of the method, directly applicable to any complex quantum system.

6.6. Towards tight impossibility and possibility results for string stability

Participants: Alain Sarlette

This is the last step of the PhD thesis of Arash Farnam under the direction of A. Sarlette at Ghent University. The aim was to study which elements are really essential in so-called “string instability” results, which exist in several variants and with several assumptions. In [15], we have significantly extended the often frequency-based linear approach, by showing how the assumptions lead to string instability also in any nonlinear systems with reasonable bandwidth. This should allow to clarify that how the problem setting must be adapted in order to obtain more positive results. In [14], we show how other elements do not help, and we clarify how the knowledge of individual vehicles’ absolute velocity is key to enable strong versions of string stability, in conjunction with PID control. Previous studies had only considered weaker versions, with PD type control. A more detailed study of string stability with absolute velocity control has also been published in [25].

6.7. Stabilization of quantum systems under continuous non-demolition measurements

Participants: Gerardo Cardona, Alain Sarlette and Pierre Rouchon

The stabilization of quantum states or quantum subspaces using feedback signals from quantum non-demolition measurements is a basic control task; in discrete-time, this is the fundamental control property shown in the first quantum feedback experiment by Serge Haroche. In continuous-time, the problem is harder. So-called Markovian feedback can stabilize some states, but in particular the quantum non-demolition eigenstates which would be marginally stable under measurements, cannot be stabilized asymptotically with this technique. Stochastic control techniques, based on feedback from a full state estimator, have been proposed and analyzed to stabilize such eigenstates, proving convergence but not much more. In [12], we prove how a relatively simple controller, feeding back Wiener noise with a gain that depends on eigenstate populations, allows to exponentially stabilize the target eigenstate. This generalizes our previous results about the qubit.

In [24], we provide a similar scheme and convergence proof for stabilizing an invariant subspace of the measurement, namely the codespace of a repetition code for quantum error correction. To the best of our knowledge there was no convergence proof so far for stabilizing such subspaces on the basis of continuous measurements.

6.8. Modified Integral Control Globally Counters Symmetry-Breaking Biases

Participants: Alain Sarlette

This is the end of the PhD thesis of Zhifei Zhang, under joint supervision of A.Sarlette at Ghent University and Zhihao Ling at ECUST Shanghai. The work [23] builds on our earlier proposal of formulating integral control on nonlinear groups as the integral of proportional correcting feedback actions: since these actions belong to a Lie algebra, they can be integrated in this vector space and applied at the current point. We here show how this controller can be modified in order to recover coordinated motion among steering-controlled vehicles, in a situation where biases would make the standard controller fail. We prove how the simple addition of the integral controller allows to recover global convergence towards the coordinated motion, restoring symmetry exactly.

6.9. Quantum Fast-Forwarding: Markov Chains and graph property testing

Participants: Alain Sarlette

This is the end of the PhD thesis of S.Apers, under supervision of A.Sarlette at Ghent University. In [11], we propose a quantum algorithmic routine, called Quantum Fast-Forwarding, which allows to simulate a Markov chain quadratically faster on a quantum computer than on a classical one. The key novelty, from an application point of view, is that we can achieve this acceleration not only for reaching the asymptotic distribution, but also for any intermediate time that one would be interested in. Such transient behaviors of Markov chains are important in algorithmic context, for instance to distinguish clusters in graphs. We explicitly work out those applications on graph properties.

6.10. Quantum Adiabatic Elimination: extension to rotating systems

Participants: Paolo Forni, Timothée Launay, Alain Sarlette and Pierre Rouchon

Adiabatic elimination is a technique to eliminate fast converging variables of a large system, while retaining their impact on slower dynamics of interest. Its most extreme form is a standard procedure when neglecting the dynamics of e.g. actuators or measurement devices in dynamical systems. In quantum systems it is particularly relevant to eliminate subsystems in tensor product structure. However, a major constraint is to obtain a reduced system in quantum form (Lindblad equations), preserving positivity and the unit trace. After having set up the framework for quantum adiabatic elimination to arbitrary order as a series expansion during the thesis of Rémi Azouit, we had worked out first- and second-order Lindblad equations only. With Paolo Forni, we have been pursuing the development of explicit formulas for higher-order cases. In [26], we present an extension of the technique for the case where the slowly decaying subsystem of interest, is subject to fast Hamiltonian dynamics. This appears e.g. in systems with significant detunings, where a description in rotating frame would lead to time-dependent equations if one does not want to neglect fast oscillating terms.

6.11. Minimizing decoherence on target in bipartite open quantum systems

Participants: Paolo Forni and Alain Sarlette

We consider a target quantum system, coupled to an auxiliary quantum system which dissipates rapidly at somewhat adjustable rates. The goal is to minimize the dissipation induced on the target system by this coupling. In [27], we use explicit model reduction formulas to express this as a quadratic optimization problem. We prove that maybe counterintuitively, when the auxiliary system dissipates along Hermitian (entropy-increasing) channels, the minimum induced dissipation is reached by maximizing the dissipation rate of the auxiliary system. This may be interpreted as a dynamical decoupling among the target system and the auxiliary one, induced not by standard Hamiltonian control acting on the target, but by noise acting on the environment. This link has been pursued with PhD student Michiel Burgelman and should lead to further results next year.

6.12. Repetition Cat Qubits for Fault-Tolerant Quantum Computation

Participants: Jérémie Guillaud and Mazyar Mirrahimi

We present a 1D repetition code based on the so-called cat qubits as a viable approach toward hardware-efficient universal and fault-tolerant quantum computation. The cat qubits that are stabilized by a two-photon driven-dissipative process exhibit a tunable noise bias where the effective bit-flip errors are exponentially suppressed with the average number of photons. We propose a realization of a set of gates on the cat qubits that preserve such a noise bias. Combining these base qubit operations, we build, at the level of the repetition cat qubit, a universal set of fully protected logical gates. This set includes single-qubit preparations and measurements, not, controlled-not, and controlled-controlled-not (Toffoli) gates. Remarkably, this construction avoids the costly magic state preparation, distillation, and injection. Finally, all required operations on the cat qubits could be performed with slight modifications of existing experimental setups.

This result was recently published in Physical Review X [16].

6.13. Experimental Implementation of a Raman-Assisted Eight-Wave Mixing Process

Participants: Mazyar Mirrahimi

Nonlinear processes in the quantum regime are essential for many applications, such as quantum-limited amplification, measurement, and control of quantum systems. In particular, the field of quantum error correction relies heavily on high-order nonlinear interactions between various modes of a quantum system. However, the required order of nonlinearity is often not directly available or weak compared to dissipation present in the system. Here, following our earlier theoretical proposal [72] we experimentally demonstrate a route to obtain higher-order nonlinearity by combining more easily available lower-order nonlinear processes, using a generalization of the Raman transition. In particular, we show a transformation of four photons of a high-Q superconducting resonator into two excitations of a superconducting transmon mode and two pump photons, and vice versa. The resulting eight-wave mixing process is obtained by cascading two fourth-order nonlinear processes through a virtual state. We expect this type of process to become a key component of hardware-efficient quantum error correction using continuous-variable error-correction codes. This work in collaboration with the group of Michel Devoret at Yale university was published in [18].

6.14. Stabilized Cat in a Driven Nonlinear Cavity: A Fault-Tolerant Error Syndrome Detector

Participants: Philippe Campagne-Ibarcq and Mazyar Mirrahimi

In quantum error correction, information is encoded in a high-dimensional system to protect it from the environment. A crucial step is to use natural, two-body operations with an ancilla to extract information about errors without causing backaction on the encoded information. Essentially, ancilla errors must not propagate to the encoded system and induce errors beyond those which can be corrected. The current schemes for achieving this fault tolerance to ancilla errors come at the cost of increased overhead requirements. An efficient way to extract error syndromes in a fault-tolerant manner is by using a single ancilla with a strongly biased noise channel. Typically, however, required elementary operations can become challenging when the noise is extremely biased. In this collaborative work with the groups of Steven Girvin and Michel Devoret at Yale University, we propose to overcome this shortcoming by using a bosonic-cat ancilla in a parametrically driven nonlinear oscillator. Such a cat qubit experiences only bit-flip noise, while the phase flips are exponentially suppressed. To highlight the flexibility of this approach, we illustrate the syndrome extraction process in a variety of codes such as qubit-based toric, bosonic-cat, and Gottesman-Kitaev-Preskill codes. Our results open a path for realizing hardware-efficient, fault-tolerant error syndrome extraction. This work was published in [21].

SPHINX Project-Team

7. New Results

7.1. Control, stabilization and optimization of heterogeneous systems

Participants: Rémi Buffe, Thomas Chambrion, Eloïse Comte, Arnab Roy, Takéo Takahashi, Jean-François Scheid, Julie Valein.

Control and optimization

The use of measures (instead of functions) as controls is usually referred to as “impulsive control”. While the theory is now well understood for finite dimensional dynamics, many questions are still open for the control of PDEs. In [19], Thomas Chambrion and his co-authors discuss the notion of solution for the impulsive control (using measures instead of functions for the control) of the general bilinear Schrödinger equations. The results are adapted in [35] to the case of potentials with high regularity. These techniques have been used to extend the celebrated obstruction to controllability by Ball, Marsden and Slemrod to the case of abstract bilinear equations with bounded potentials [33] and the Klein-Gordon equation [20]. Other obstructions to controllability (preservation of regularity) have been investigated for the Gross-Pitaiewski equation with unbounded potentials [34].

In [15], an optimal control problem for groundwater pollution due to agricultural activities is considered, the objective being the optimization of the trade-off between the fertilizer use and the cleaning costs. The spread of the pollution is modeled by a convection-diffusion-reaction equation. We are interested in the buffer zone around the captation well and we determine its optimal size.

In [44], Eduardo Cerpa, Emmanuelle Crépeau and Julie Valein study the boundary controllability of the Korteweg-de Vries equation on a tree-shaped network, with less controls than equations.

In [27], Jérôme Lohéac and Takéo Takahashi study the locomotion of a ciliated microorganism in a viscous incompressible fluid. They use the Blake ciliated model: the swimmer is a rigid body with tangential displacements at its boundary that allow it to propel in a Stokes fluid. This can be seen as a control problem: using periodical displacements, is it possible to reach a given position and a given orientation? They are interested in the minimal dimension d of the space of controls that allows the microorganism to swim. Their main result states the exact controllability with $d = 3$ generically with respect to the shape of the swimmer and with respect to the vector fields generating the tangential displacements. The proof is based on analyticity results and on the study of the particular case of a spheroidal swimmer.

In [31], Arnab Roy and Takéo Takahashi study the controllability of a fluid-structure interaction system. They consider a viscous and incompressible fluid modeled by the Boussinesq system and the structure is a rigid body with arbitrary shape which satisfies Newton’s laws of motion. They assume that the motion of this system is bidimensional in space. They prove the local null controllability for the velocity and temperature of the fluid and for the position and velocity of the rigid body for a control acting only on the temperature equation on a fixed subset of the fluid domain.

Rémi Buffe and Ludovick Gagnon consider N manifolds without boundary that intersect each other. They assume that the speed of propagation on each manifold is different, which implies that the Snell conditions applies at the interface. They give sufficient geometric conditions to ensure the controllability with distributed controls on $N - 1$ manifolds.

Stabilization

In [17], Lucie Baudouin, Emmanuelle Crépeau and Julie Valein study the exponential stability of the nonlinear Korteweg-de Vries equation with boundary time-delay feedback. Two different methods are employed: a Lyapunov functional approach (allowing to have an estimation on the decay rate, but with a restrictive assumption on the length of the spatial domain of the KdV equation) and an observability inequality approach, with a contradiction argument (for any non-critical lengths but without estimation on the decay rate).

In [55], Julie Valein shows the semi-global exponential stability of the nonlinear Korteweg-de Vries equation in the presence of a delayed internal feedback, for any lengths, in the case where the weight of the feedback with delay is smaller than the weight of the feedback without delay. In the case where the support of the feedback without delay is not included in the support of the feedback with delay, a local exponential stability result is proved if the weight of the delayed feedback is small enough.

Optimization
J.F. Scheid, V. Calesti (PhD Student) and I. Lucardesi study an optimal shape problem for an elastic structure immersed in a viscous incompressible fluid. They want to establish the existence of an optimal elastic domain associated with an energy-type functional for a Stokes-Elasticity system. We want to find an optimal reference domain (the domain before deformation) for the elasticity problem that minimizes an energy-type functional. This problem is concerned with 2D geometry and is an extension of the work of [113] for a 1D problem. The optimal domain is seeking in a class of admissible open sets defined with a diffeomorphism of a given domain. The main difficulty lies on the coupling between the Stokes problem written in a eulerian frame and the linear elasticity problem written in a lagrangian form. The shape derivative of the energy-type functional is also aimed to be determined in order to numerically obtain an optimal elastic domain. This work is in progress.

7.2. Direct and Inverse problems for heterogeneous systems

Participants: Rémi Buffe, Imene Djebour, David Dos Santos Ferreira, Ludovick Gagnon, Alexandre Munnier, Julien Lequeurre, Karim Ramdani, Takéo Takahashi, Jean-Claude Vivalda.

Direct problems
In [22], Imene Djebour and Takéo Takahashi consider a fluid–structure interaction system composed by a three-dimensional viscous incompressible fluid and an elastic plate located on the upper part of the fluid boundary. They use here Navier-slip boundary conditions instead of the standard no-slip boundary conditions. The main results are the local in time existence and uniqueness of strong solutions of the corresponding system and the global in time existence and uniqueness of strong solutions for small data and if one assumes the presence of frictions in the boundary conditions.

In [42], Mehdi Badra (University of Toulouse) and Takéo Takahashi analyze a bi-dimensional fluid-structure interaction system composed by a viscous incompressible fluid and a beam located at the boundary of the fluid domain. The main result is the existence and uniqueness of strong solutions for the corresponding coupled system. The proof is based on a the study of the linearized system and a fixed point procedure. In particular, they show that the linearized system can be written with a Gevrey class semigroup. The main novelty with respect to previous results is that they do not consider any approximation in the beam equation.

In [18], Muriel Boulakia (Sorbonne University), Sergio Guerrero (Sorbonne University) and Takéo Takahashi consider a system modeling the interaction between a viscous incompressible fluid and an elastic structure. The fluid motion is represented by the classical Navier–Stokes equations while the elastic displacement is described by the linearized elasticity equation. The elastic structure is immersed in the fluid and the whole system is confined into a general bounded smooth three-dimensional domain. The main result is the local in time existence and uniqueness of a strong solution of the corresponding system.

In [28], Debayan Maity (TIFR Bangalore), Jorge San Martin (University of Chile), Takéo Takahashi and Marius Tucsnak (University of Bordeaux) study the interaction of surface water waves with a floating solid constraint to move only in the vertical direction. They propose a new model for this interaction, taking into consideration the viscosity of the fluid. This is done supposing that the flow obeys a shallow water regime (modeled by the viscous Saint-Venant equations in one space dimension) and using a Hamiltonian formalism. Another contribution of this work is establishing the well-posedness of the obtained PDEs/ODEs system in function spaces similar to the standard ones for strong solutions of viscous shallow water equations. Their well-posedness results are local in time for any initial data and global in time if the initial data are close (in appropriate norms) to an equilibrium state. Moreover, they show that the linearization of the system around an equilibrium state can be described, at least for some initial data, by an integro-fractional differential equation related to the classical Cummins equation and which reduces to the Cummins equation when the viscosity vanishes and the fluid is supposed to fill the whole space. Finally, they describe some numerical tests, performed on the original nonlinear system, which illustrate the return to equilibrium and the influence of the viscosity coefficient.

In [30], Benjamin Obando and Takéo Takahashi consider the motion of a rigid body in a viscoplastic material. This material is modeled by the 3D Bingham equations, and the Newton laws govern the displacement of the rigid body. The main result is the existence of a weak solution for the corresponding system. The weak formulation is an inequality (due to the plasticity of the fluid), and it involves a free boundary (due to the motion of the rigid body). They approximate it by regularizing the convex terms in the Bingham fluid and by using a penalty method to take into account the presence of the rigid body.

In [23], Alexandre Munnier and his co-authors consider the dynamics of several rigid bodies immersed in a perfect incompressible fluid. We show that this dynamics can be modelized by a second order ODE whose coefficients depend on the vorticity and the circulation of the fluid around the bodies. This formulation permits to point out the geodesic nature of the solutions, the added mass effect, the gyroscopic effects and the Kutta-Joukowski-type lift forces.

In [24], Julien Lequeurre and his co-authors study an unsteady nonlinear fluid–structure interaction problem. We consider a Newtonian incompressible two-dimensional flow described by the Navier-Stokes equations set in an unknown domain depending on the displacement of a structure, which itself satisfies a linear wave equation or a linear beam equation. The fluid and the structure systems are coupled via interface conditions prescribing the continuity of the velocities at the fluid–structure interface and the action-reaction principle. We prove existence of a unique local in time strong solution. In the case of the wave equation or a beam equation with inertia of rotation, this is, to our knowledge the first result of existence of strong solutions for which no viscosity is added. One key point, is to use the fluid dissipation to control, in appropriate function spaces, the structure velocity.

J.F. Scheid and M. Bouguezzi (PhD student) in collaboration with D. Hilhorst and Y. Miyamoto work on the convergence of the solution of the one-phase Stefan problem in one-space dimension to a self-similar profile. The evolutional self-similar profile is viewed as a stationary solution of a Stefan problem written in a self-similar coordinates system. The proof of the convergence relies on the construction of sub and super-solutions for which it must be proved that they both tend to the same function. It remains to show that this limiting function actually corresponds to the self-similar solution of the original Stefan problem. This work is in progress.

Rémi Buffe, Ludovick Gagnon *et al.* obtain the exponential decay of the solutions of coupled wave equations with a transmission condition at the interface and with a viscoelastic damping term. They prove that the exponential decay is obtained if the support of the viscoelastic term satisfies the uniform escaping geometry condition. They also deal with the case where the damping term touches the interface.

Inverse problems

In [43], the authors are interested in the homogenization of time-harmonic Maxwell's equations in a composite medium with periodically distributed small inclusions of a negative material. Here a negative material is a material modelled by negative permittivity and permeability. Due to the sign-changing coefficients in the equations, it is not straightforward to obtain uniform energy estimates to apply the usual homogenization techniques. The analysis is based on a precise study of two associated scalar problems: one involving the sign-changing permittivity with Dirichlet boundary conditions, another involving the sign-changing permeability with Neumann boundary conditions. For both problems, we obtain a criterion on the physical parameters ensuring uniform invertibility of the corresponding operators as the size of the inclusions tends to zero. Then we use the results obtained for the scalar problems to derive uniform energy estimates for Maxwell's system.

In [37], Jean-Claude Vivalda and his co-authors prove that the class of continuous-time systems who are strongly differentially observable after time sampling is everywhere dense in the set of pairs (f, h) where f is a (parametrized) vector field given on a compact manifold and h is an observation function.

In [47], using a partial boundary measurement, Jean-Claude Vivalda and his co-authors design an observer for a system that models a desalination device; this observer being used to make an output tracking trajectory.

Rémi Buffe, David Dos Santos Ferreira and Ludovick Gagnon obtain an estimate on the magnetic Laplacian with sharp dependance on the power of the zeroth and first order potential and close to sharp norm of these potentials. This estimate is related to the observability inequality for the wave equation and to the cost of the control.

7.3. Numerical analysis and simulation of heterogeneous systems

Participant: Xavier Antoine.

Acoustics

Artificial boundary conditions: while high-order absorbing boundary conditions (HABCs) are accurate for smooth fictitious boundaries, the precision of the solution drops in the presence of corners if no specific treatment is applied. In [29], the authors present and analyze two strategies to preserve the accuracy of Padé-type HABCs at corners: first by using compatibility relations (derived for right angle corners) and second by regularizing the boundary at the corner. Exhaustive numerical results for two- and three-dimensional problems are reported in the paper. They show that using the compatibility relations is optimal for domains with right angles. For the other cases, the error still remains acceptable, but depends on the choice of the corner treatment according to the angle.

Domain decomposition : in [49], Xavier Antoine and his co-authors develop the first application of the optimized Schwarz domain decomposition method to aeroacoustics. Highly accurate three-dimensional simulations for turbofans are conducted through a collaboration with Siemens (ongoing CIFRE Ph.D. Thesis of Philippe Marchner). In [26], the authors propose a new high precision IGA B-Spline approximation of the high frequency scattering Helmholtz problem, which minimizes the numerical pollution effects that affect standard Galerkin finite element approaches.

Underwater acoustics

New adiabatic pseudo-differential models as well as their numerical approximation are introduced in [53] for the simulation of the propagation of wave fields in underwater acoustics. In particular, the calculation of gallery modes is shown to be accurately obtained. This work is related to a new collaboration with P. Petrov from the V.I. Il'ichev Pacific Oceanological Institute, Vladivostok, Russia.

Quantum theory

With E. Lorin, Xavier Antoine proposes in [13] an optimization technique of the convergence rate of relaxation Schwarz domain decomposition methods for the Schrödinger equation. This analysis is based on the use of microlocal analysis tools. Convergence proofs are given in [11] for the real-time Schrödinger equation with optimized transmission conditions. We extend these results to the case of multiple subdomains in [13].

In [52], the authors analyze the convergence and stability in of a discretization scheme for the linear Schrödinger equation with artificial boundary conditions.

In [39], Xavier Antoine and his co-authors develop an implementation of the PML technique in the framework of Fourier pseudo-spectral approximation schemes for the fast rotating Gross-Pitaevskii equation. This is the first work related to the international Inria team BEC2HPC, associated with China (https://team.inria.fr/bec2hpc/).

In [12], Antoine and his co-authors develop new Fourier pseudo-spectral schemes including a PML for the dynamics of the Dirac equation. The implementation of the method leads to the possibility of simulating complex quantum situations. In [38], the authors extend the approximation to the curved static Dirac equation. The goal is to be able to better understand quantum phenomena related to the charge carriers in strained graphene, with potential long term applications for designing quantum computers. This is a collaboration with E. Lorin (Carleton University), F. Fillion-Gourdeau and S. Mac Lean from the Institute for Quantum Computing, University of Waterloo.

Fractional PDE

In [32], with J. Zhang and D. Li, Xavier Antoine is interested in the development and analysis of fast second-order schemes to simulate the nonlinear time fractional Schrödinger equation in unbounded domains.

The authors propose in [14] the construction of PML operators for a large class of space fractional PDEs in one- and two-dimensions. The specific case of the fractional laplacian is carefully considered.

Xavier Antoine and Emmanuel Lorin are interested in [40] in the problem of building fast and robust linear algebra algorithms based on the discretization of the Cauchy integral formula used to represent the power matrix. Applications related to stationary PDEs are presented, with possibly randomly perturbed potentials. Differential doubly preconditioned iterative schemes are investigated in details in [41] to evaluate the power, and more generally functions, of matrices.

Error estimates of a semi-implicit ALE scheme for the one-phase Stefan problem. J.F. Scheid, M. Bouguezzi (PhD student) and D. Hilhorst study the convergence with error estimates of an Arbitrary-Lagrangian-Eulerian (ALE) scheme for the classical one-phase Stefan problem. Despite Stefan problems as well as ALE techniques are well-known in the mathematical litterature for many decades, surprisingly there is no global result on convergence (with error estimates) for fully space-time discretized scheme based on ALE formulations. The main difficulty lies on the unbounded behavior of the exact (and approximate) free boundary. Stability results have already been obtained for a time-discretized scheme (and continuous in space) for the one-space dimension case.

Chaotic advection in a viscous fluid under an electromagnetic field. J.F. Scheid, J.P. Brancher and J. Fontchastagner study the chaotic behavior of trajectories of a dynamical system arising from a coupling system beetwen Stokes flow and an electromagnetic field. They consider an electrically conductive viscous fluid crossed by a uniform electric current. The fluid is subjected to a magnetic field induced by the presence of a set of magnets. The resulting electromagnetic force acts on the conductive fluid and generates a flow in the fluid. According to a specific arrangement of the magnets surrounding the fluid, vortices can be generated and the trajectories of the dynamical system associated to the stationary velocity field in the fluid may have chaotic behavior. The aim of this study is to numerically show the chaotic behavior of the flow for the proposed disposition of the magnets along the container of the fluid. The flow in the fluid is governed by the Stokes equations with the Laplace force induced by the electric current and the magnetic field. An article is in preparation.

TRIPOP Project-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 compression waves (solitary waves or fronts) or localized 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 [8], 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-Lipschitz 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 addition, G.J. has developed a theoretical method to analyze impacts in homogeneous granular chains with KK dissipation. The idea is to use the exponent α of the contact force as a parameter and derive simpler dynamical equations through an asymptotic analysis, in the limit when α approaches unity and long waves are considered. In that case, different continuum limits of the granular chain can be obtained. When the contact damping constant remains of order unity, wave profiles are well approximated by solutions of a viscous Burgers equation with logarithmic nonlinearity. For small contact damping, dispersive effects must be included and the continuum limit corresponds to a KdV-Burgers equation with logarithmic nonlinearity. By studying traveling wave solutions to these partial differential equations, we obtain analytical approximations of wave profiles such as compression fronts. We observe that these approximations remain meaningful for the classical exponent $\alpha = 3/2$. Indeed, they are close to exact wave profiles computed numerically for the KK model, using both dynamical simulations (response of the chain to a compression by a piston) and the Newton method (computation of exact traveling waves by a shooting method). In addition, in analogy with the Rankine-Hugoniot conditions for hyperbolic systems, we relate the asymptotic states of the KK model (for an infinite granular chain) to the velocity of a propagating front. These results are described in an article in preparation.

6.2. 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.

6.3. Hybrid Differential Algebraic equations

Participants: Vincent Acary, Bernard Brogliato, Alexandre Rocca.

In [18], [21], we study differential algebraic equations with constraints defined in a piecewise manner using a conditional statement. Such models classically appear in systems where constraints can evolve in a very small time frame compared to the observed time scale. The use of conditional statements or hybrid automata are a powerful way to describe such systems and are, in general, well suited to simulation with event driven numerical schemes. However, such methods are often subject to chattering at mode switch in presence of sliding modes, or can result in Zeno behaviours. In contrast, the representation of such systems using differential inclusions and method from non-smooth dynamics are often closer to the physical theory but may be harder to interpret. Associated time-stepping numerical methods have been extensively used in mechanical modelling with success and then extended to other fields such as electronics and system biology. In a similar manner to the previous application of non-smooth methods to the simulation of piecewise linear ODEs, non-smooth event-capturing numerical scheme are applied to piecewise linear DAEs. In particular, the study of a 2-D dynamical system of index-2 with a switching constraint using set-valued operators, is presented.

6.4. Numerical analysis of multibody mechanical systems with constraints

This scientific theme concerns the numerical analysis of mechanical systems with bilateral and unilateral constraints, with or without friction [1]. They form a particular class of dynamical systems whose simulation requires the development of specific methods for analysis and dedicated simulators [57].

6.4.1. Numerical solvers for frictional contact problems.

Participants: Vincent Acary, Maurice Brémond, Paul Armand.

In [34], 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.

Recently, new developments have been carried out on two new applications of well-known numerical methods in Optimization:

- *Interior point methods* With the visit of Paul Armand, Université de Limoges, we co-supervise a M2 internship, Maksym Shpakovych on the application of interior point methods for quadratic problem with second-order cone constraints. The results are encouraging and a publication in computational mechanics is in progress.
- *Alternating Direction Method of Multipliers*. In collaboration with Yoshihiro Kanno, University of Tokyo, the use of the Alternating Direction Method of Multipliers (ADMM) has been adapted to the discrete frictional contact problems. With the help of some acceleration and restart techniques for first-order optimization methods and a residual balancing technique for adapting the proximal penalty parameter, the method proved to be efficient and robust on our test bench examples. A publication is also in preparation on this subject.

6.4.2. Modeling and numerical methods for frictional contact problems with rolling resistance

Participants: Vincent Acary, Franck Bourrier.

In [19], the Coulomb friction model is enriched to take into account the resistance to rolling, also known as rolling friction. Introducing the rolling friction cone, an extended Coulomb's cone and its dual, a formulation of the Coulomb friction with rolling resistance as a cone complementarity problem is shown to be equivalent to the standard formulation of the Coulomb friction with rolling resistance. Based on this complementarity formulation, the maximum dissipation principle and the bi-potential function are derived. Several iterative numerical methods based on projected fixed point iterations for variational inequalities and block-splitting techniques are given. The efficiency of these method strongly relies on the computation of the projection onto the rolling friction cone. In this article, an original closed-form formulae for the projection on the rolling friction cone is derived. The abilities of the model and the numerical methods are illustrated on the examples of a single sphere sliding and rolling on a plane, and of the evolution of spheres piles under gravity.

6.4.3. Finite element modeling of cable structures

Participants: Vincent Acary, Charlélie Bertrand.

Standard finite element discretization for cable structures suffer from several drawbacks. The first one is related to the mechanical assumption that the cable can not support compression. Standard formulations do not take into account this assumption. The second drawback comes from the high stiffness of the cable model when we deal with large lengths with high Young modulus such as cable ropeways installations. In this context, standard finite element applications cannot avoid compressive solutions and have huge difficulties to converge. In a forthcoming paper, we propose to a formulation based on a piecewise linear modeling of the cable constitutive behavior where the elasticity in compression is canceled. Furthermore, a dimensional analysis help us to formulate a problem that is well-balanced and the conditioning of the problem is diminished. The finite element discretization of this problem yields a robust method where convergence is observed with the number of elements and the nonlinear solver based on nonsmooth Newton strategy is converging up to tight tolerances. The convergence with the number of element allows one to refine the mesh as much as we want that will be of utmost importance for applications with contact and friction. Indeed, a fine discretization with respect to the whole length of the cable will be possible in the contact zone.

6.4.4. Well-posedness of the contact problem

We continue in [3] the analysis of the so-called contact problem for Lagrangian systems with bilateral and unilateral constraints, with set-valued Coulomb's friction. The problem that is analysed this time concerns sticking contacts (in both the normal and the tangential directions), *i.e.*, does there exist a solution (possibly unique) to the contact problem (that takes the form of a complementarity problem) when all contacts are sticking ? An algorithm is proposed that allows in principle to compute solutions. We rely strongly on results of existence and uniqueness of solutions to variational inequality of the second kind, obtained in the team some years ago. Let us note also the erratum/addendum of the monograph [45] in [17], which is regularly updated.

6.5. Analysis and Control of Set-Valued Systems

Participants: Bernard Brogliato, Christophe Prieur, Vincent Acary.

6.5.1. Robust sliding-mode control: continuous and discrete-time

The implicit method for the time-discretization of set-valued sliding-mode controllers was introduced in [29], [31]. The backstepping approach is used in [9] to design a continuous-time and a discrete-time nested set-valued controller that is able to reject unmatched disturbances (a problem that is known to be tough in the sliding-mdoe control community). In [13], [10] we continue 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). The discrete-time analysis of the twisting and the super-twisting algorithms are tackled in [7], [4].

6.5.2. Analysis of set-valued Lur'e dynamical systems

Lur'e systems are very popular in the Automatic Control field since their introduction by Lur'e in 1944. In [5] we propose a very complete survey/tutorial on the set-valued version of such dynamical systems (in finite dimension) which mainly consist of the negative feedback interconnection of an ODE with a maximal monotone set-valued operator. The first studies can be traced back to Yakubpovich in 1963 who analysed the stability of a linear time invariant system with positive real constraints, in negative feedback connection with a hysteresis operator. About 600 references are analysed from the point of view of the mathematical formalisms (Moreau's sweeping process, evolution variational inequalities, projected dynamical systems, complementarity dynamical systems, maximal monotone differential inclusions, differential variational inequalities), the relationships between these formalisms, the numerous fields of application, the well-posedness issues (existence, uniqueness and continuous dependence of solutions), and the stability issues (generalized equations for fixed points, Lyapunov stability, invariance principles).

6.5.3. Optimal control of LCS

The quadratic and minimum time optimal control of LCS as in (6) is tackled in [14], [12]. 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).

6.6. Dissipative systems

Participant: Bernard Brogliato.

The third edition of the book Dissipative Systems Analysis and Control has been released https://www.springer.com/gp/book/9783030194192. Also a short proof of equivalence of side conditions for strictly positive real (SPR) transfer functions is done in [6], closing a long debate in the Automatic Control community about the characterization of SPR transfer matrices.

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, applied 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 [41], 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 [14], 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 [77].

7.1.2. Nonlinear fixed point methods to compute joint spectral raddi of nonnegative matrices

Participant: Stéphane Gaubert.

In [21], 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).

7.1.3. Probabilistic and max-plus approximation of Hamilton-Jacobi-Bellman equations

Participant: Marianne Akian.

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 [36], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [92], [98] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [70] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [37] and [27], we improved 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 studied the convergence and obtain error estimates when the parameters and the value function are bounded.

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 [99], [100], the stochastic max-plus scheme proposed by Zheng Qu [108], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [105], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [55], the probabilistic numerical method of Fahim, Touzi and Warin [70]. We propose to associate and compare these methods in order to solve more general structures.

In a first work [35], see also [24], 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. More recently, we study generalizations of these algorithms to the case of stochastic optimal control problems.

In a recent work, we introduce and study an entropic relaxation of the Nested Distance introduced by Pflug [106].

7.1.5. A variance reduction deflated value iteration algorithm to solve ergodic games

Participants: Marianne Akian, Stéphane Gaubert, Omar Saadi.

Recently, Sidford et al. introduced in [116] a variance reduced value iteration algorithm to solve discounted Markov decision processes. In [25], in a joint work work with Zheng Qu (Hong Kong University), we extended this algorithm to the ergodic (mean payoff) case, and also to the two-player case, exploiting techniques from non-linear spectral theory [39] and variational analysis. The deterministic version of this algorithm also yields a new method (alternative to relative value iteration) to solve ergodic problems.

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 ordered vector spaces that preserve or reverse the order structure. A bijective map that preserves the order in both directions is called an order isomorphism, and one that reverse the order in both directions is called an order antimorphism. These maps are closely related to the isometries of the Hilbert and Thompson metrics on the interior of the cone of positive elements.

The study of the order isomorphisms of an ordered vector space 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 affine 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 positive cone is the convex hull of its extreme rays, which is overly restrictive in infinite dimension.

In a recent preprint [34], we broaden the scope of these results, requiring only very mild assumptions, namely that the spaces involved are *complete order unit spaces*. These are ordered vector spaces whose cone of positive elements is Archimedean, and that have an order unit, such that the norm induced by this order unit is complete. We show that the existence of an order isomorphism between two such spaces implies that they are in fact linearly isomorphic as ordered vector spaces.

In addition, we introduce a necessary and sufficient criterion for all order isomorphisms on a complete order-unit space to be affine. This criterion is in terms of the geometry of the dual cone. In the current setting, the dual cone has a cross-section called the state space, whose extreme points are called pure states. The closure of the set of pure states is known as the pure state space. The criterion is then that the union of the supports of the affine dependencies supported by the pure state space is dense in the pure state space.

7.2.2. Generalization of the Hellinger distance

Participant: Stéphane Gaubert.

In [58] (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.

7.2.3. Spectral inequalities for nonnegative tensors and their tropical analogues

Participant: Stéphane Gaubert.

In [30] (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

Participant: Xavier Allamigeon.

This work is joint with Ricardo Katz (Conicet, Argentina) and Pierre-Yves Strub (LIX, Ecole Polytechnique).

In [54], 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.

The most recent advances on the project are described in the software section.

7.3.2. Tropical totally positive matrices and planar networks

Participant: Stéphane Gaubert.

In [79] (joint work with Adi Niv) we characterized 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 showed 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. A fundamental property of classical totally positive matrices is their representation as weight matrices of planar network; in the recent work [31], we studied the tropical analogue of this property.

7.3.3. Linear algebra over systems

Participants: Marianne Akian, Stéphane Gaubert.

In a joint work with Louis Rowen (Univ. Bar Ilan), we study linear algebra and convexity properties over "systems". The latter provide a general setting encompassing extensions of the tropical semifields and hyperfields. A first account of this work was presented by Marianne Akian and Louis Rowen at the SIAM conference on applied algebraic geometry, in Bern.

7.3.4. Ambitropical convexity and Shapley retracts

Participants: Marianne Akian, Stéphane Gaubert.

Closed tropical convex cones are the most basic examples of modules over the tropical semifield. They coincide with sub-fixed-point sets of Shapley operators – dynamic programming operators of zero-sum games. We study a larger class of cones, which we call "ambitropical" as it includes both tropical cones and their duals. Ambitropical cones can be defined as lattices in the order induced by Rn. Closed ambitropical cones are precisely the fixedpoint sets of Shapley operators. They are characterized by a property of best co-approximation arising from the theory of nonexpansive retracts of normed spaces. Finitely generated ambitropical cones arise when considering Shapley operators of deterministic games with finite action spaces. Finitely generated ambitropical cones are special polyhedral complexes whose cells are alcoved poyhedra, and locally, they are in bijection with order preserving retracts of the Boolean cube This is a joint work with Sara Vannucci (invited PhD student from Salerno university). A first account of this work was presented by Stéphane Gaubert at the JAMI Workshop, Riemann-Roch theorem in characteristic one and related topics, in Baltimore.

7.3.5. Volume and integer points of tropical polytopes

Participant: Stéphane Gaubert.

We investigate in [20] (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 $\mathrm{P} = \mathrm{NP}$.

7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

7.4.1. Tropicalization of semidefinite programming and its relation with stochastic games

Participants: Xavier Allamigeon, Stéphane Gaubert.

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.

The PhD thesis of Mateusz Skomra [118] dealt about 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 studied 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 [52] (now accepted for publication in Disc. Comp. Geom), with further results in the PhD thesis [118].

We showed in [53] 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, [114] disproved this conjecture. In [15], 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 [52] and [53].

In [50] and [118], we exploited 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.

7.4.2. Tropical polynomial systems and colorful interior of convex bodies

Participants: Marianne Akian, Marin Boyet, Xavier Allamigeon, Stéphane Gaubert.

We studied 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 were investigated, as well as the relation between tropical colorful interiors and support vector machines. These results were presented by M. Boyet at the SIAM AG conference in Bern.

7.4.3. Universal approximation theorems by log-sum-exp neural networks

Participant: Stéphane Gaubert.

This is a joint work with Giuseppe Calafiore and Corrado Possieri (Torino).

We establish universal properties of functions by neural networks with log-sum-exp activation functions, first for convex functions [19], and then in general [29]. Some consequences, including approximation by subtraction free rational expressions, are derived.

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 ([65]) gave a spectral interpretation of the zeroes of the Riemann zeta function involving the action of $\mathbb{R}_+^*$ on the sector $X = \mathbb{Q}_+^\times \setminus \mathbb{A}_\mathbb{Q}/\widehat{\mathbb{Z}}^\times$ of the adele class space $\mathbb{A}_\mathbb{Q}/\mathbb{Q}^*$ of the field of rational numbers. In [66], [68], 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 $\mathbb{Q}(\imath\sqrt{3})$. In particular, during this year, we showed that the semiring of convex polygons introduced for those cases satisfies a sublte arithmetical universal property. These results are presented in the accepted in *Journal of Number Theory* article [111]. In a further work, developed this year, I extended this construction, dealing now with number fields K with narrow class number 1, this generalization will rely on the universal property discovered this year and on the extensive use of Shintani's unit theorem. Here again tropical algebra play a crucial role in the geometrical constructions.

7.5.2. Duality between tropical modules and congruences

Participants: Stéphane Gaubert, Aurélien Sagnier.

In a joint work with Éric Goubault (LIX, École polytechnique), we establish a duality theorem between congruences and modules over tropical semifields.

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 [71], 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. [83]). 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 the article [22], 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 emergency call centers

Participants: Xavier Allamigeon, Marin Boyet, Baptiste Colin, 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 (PFAU, "Plate forme d'appels d'urgence") 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 [46], [47], [59]. In 2019, with four students of École polytechnique, Céline Moucer, Julia Escribe, Skandère Sahli and Alban Zammit, we performed case studies, showing the improvement brought by the two level filtering procedure.

Moreover, in 2019, this work was extended to encompass the handling of health emergency calls, with a new collaboration, involving responsibles from the four services of medical emergency aid of Assistance Publique – Hôpitaux de Paris (APHP), i.e., with SAMU75, 92, 93, 94, in the framework of a project led by Dr. Christophe Leroy from APHP. As part of his PhD work, Marin Boyet developed Petri net models capturing the characteristic of the centers (CRRA) handling emergency calls the SAMU, in order to make dimensioning recommendations.

7.6.2. Game theory and optimization methods for decentralized electric systems

Participants: Stéphane Gaubert, Paulin Jacquot.

This work is in collaboration with Nadia Oudjane, Olivier Beaude and Cheng Wan (EDF Lab).

The PhD work of Paulin Jacquot concerns the application of game theory and distributed optimization techniques to the operation of decentralized electric systems, and in particlar to the management of distributed electric consumption flexibilities. We start by adopting the point of view of a centralized operator in charge of the management of flexibilities for several agents. We provide a distributed and privacy-preserving algorithm to compute consumption profiles for agents that are optimal for the operator. In the proposed method, the individual constraints as well as the individual consumption profile of each agent are never revealed to the operator or the other agents [33] [28]. A patent related to this method has been submitted [89].

Then, in a second model, we adopt a more decentralized vision and consider a game theoretic framework for the management of consumption flexibilities. This approach enables, in particular, to take into account the strategic behavior of consumers. Individual objectives are determined by dynamic billing mechanisms, which is motivated by the modeling of congestion effects occurring on time periods receiving a high electricity load from consumers. A relevant class of games in this framework is given by atomic splittable congestion games. We obtain several theoretical results on Nash equilibria for this class of games, and we quantify the efficiency of those equilibria by providing bounds on the price of anarchy. We address the question of the decentralized computation of equilibria in this context by studying the conditions and rates of convergence of the best response and projected gradients algorithms [91], [88].

A fruitful collaboration with Cheng Wan (EDF Lab) led to the third part of this PhD thesis. In this part, we consider an operator dealing with a very large number of players, for which evaluating the equilibria in a congestion game will be difficult. To address this issue, we give approximation results on the equilibria in congestion and aggregative games with a very large number of players, in the presence of coupling constraints. These results, obtained in the framework of variational inequalities and under some monotonicity conditions, can be used to compute an approximate equilibrium, solution of a small dimension problem [32]. In line with the idea of modeling large populations, we consider nonatomic congestion games with coupling constraints, with an infinity of heterogeneous players: these games arise when the characteristics of a population are described by a parametric density function. Under monotonicity hypotheses, we prove that Wardrop equilibria of such games, given as solutions of an infinite dimensional variational inequality, can be approximated by symmetric Wardrop equilibria of auxiliary games, solutions of low dimension variational inequalities. Again, those results can be the basis of tractable methods to compute an approximate Wardrop equilibrium in a nonatomic infinite-type congestion game [33]. Last, in a collaboration with Hélène Le Cadre, Cheng Wan and Clémence Alasseur, we consider a game model for the study of decentralized peer-to-peer energy exchanges between a community of consumers with renewable production sources. We study the generalized equilibria in this game, which characterize the possible energy trades and associated individual consumptions. We compare the equilibria with the centralized solution minimizing the social cost, and evaluate the efficiency of equilibria through the price of anarchy [23].

Paulin Jacquot defended his PhD on December 5, 2019 at Ecole polytechnique [90].

VALSE Project-Team

7. New Results

7.1. Stabilization of multistable systems

Participants: Rosane Ushirobira, Denis Efimov.

The problem of robust stabilization of affine nonlinear multistable systems with respect to disturbance inputs was studied in [29]. The results are obtained using the framework of input-to-state stability and integral input-to-state stability for systems with multiple invariant sets. The notions of corresponding control Lyapunov functions as well as the small control property are extended within the multistability framework. It is verified that the universal control formula can be applied. In a similar vein, input-to-state stability and stabilization of passive multistable systems were investigated in [53].

7.2. Robustness of homogeneous systems

Participants: Andrey Polyakov, Denis Efimov.

In [32], we studied the finite-time stability of a class of nonlinear systems $\dot{x} = f(x) = H(x)b(x)$, where H is homogeneous and b is bounded. We defined the homogeneous extension of the non-homogeneous function f and used this extension to prove that, under some conditions on b, if the system $\dot{x} = f(x)$ is globally asymptotically stable, then it is finite-time stable. In [31], a theoretical basement of the previous result has been given showing robust stability of the system $\dot{x} = f(x) = H(x)b(x)$ by considering b as a perturbation.

7.3. Finite-time control and estimation in chemostat

Participants: Denis Efimov, Andrey Polyakov.

In [34], the problem of robust stabilization of the concentration of two different species competing for a single limiting substrate was addressed. Such a stabilization is performed by means of discontinuous feedback control laws that ensure coexistence of all species. The control laws are designed considering bounded uncertainties on the kinetic rates and full state measurements. The problem of robust finite-time estimation of the state for a chemostat was considered in [35].

7.4. LKF for neutral type time-delay systems

Participant: Denis Efimov.

The problem of existence of a Lyapunov-Krasovskii functional (LKF) for nonlinear neutral type time-delay systems was revisited in [37] considering the uniform stability analysis and the LKF in a Sobolev space of absolutely continuous functions with bounded derivatives.

7.5. Finite-time/Fixed-time control of PDEs

Participant: Andrey Polyakov.

The paper [40] deals with continuous boundary time-varying feedbacks for fixed-time stabilization of constant-parameter reaction-diffusion systems. IT was shown that the time of convergence can be prescribed and is independent of the initial condition of the system. The design of time-varying feedbacks was carried out by using the backstepping approach for which suitable characterizations for time-varying kernels were derived. The work [39] considered the problem of local finite-time stabilization of the viscous Burgers equation. A boundary switched linear control with state dependent switching law was designed based on the backstepping approach. The strategy builds on discontinuous kernels, which render the control function to be piecewise continuous. It was proven that such a control stabilizes locally the viscous Burgers equation and that the settling time depends on initial conditions.

7.6. Interval prediction for LPV systems

Participant: Denis Efimov.

The problem of behaviour prediction for linear parameter-varying (LPV) systems was considered in the interval framework in [41]. It was assumed that the system is subject to uncertain inputs and the vector of scheduling parameters is unmeasurable, but all uncertainties take values in a given admissible set. Then an interval predictor was designed and its stability was guaranteed applying Lyapunov function with a novel structure. The conditions of stability were formulated in the form of linear matrix inequalities. Efficiency of the theoretical results was demonstrated in the application to safe motion planning for autonomous vehicles (see videos of numeric experiments).

7.7. Finite-time/Fixed-time stability and stabilization

Participants: Andrey Polyakov, Rosane Ushirobira.

In [33], we studied the issues of prescribed-time stabilization of a chain of integrators of arbitrary length, that can be either pure (i.e. with no disturbance) or perturbed. The feedback law proposed by Song et al. was revisited, and it was shown that by an appropriately recast within the framework of time-varying homogeneity it can stabilize the system in a prescribed time. Characterizations (necessary and sufficient conditions) of finite-time and fixed-time stability of evolution inclusions in Banach spaces were presented in [44] in terms of Lyapunov functionals.

7.8. Robust stability analysis for Persidskii systems

Participant: Denis Efimov.

A class of generalized nonlinear Persidskii systems was considered in [36]. The conditions of input-to-state and integral input-to-state stability were established, which can be checked using linear matrix inequalities. The issues of discretization of this class of dynamics were analyzed using the Euler methods. The proposed theory was applied to a Lotka-Volterra model.

7.9. Design of a distributed finite-time observer

Participants: Denis Efimov, Rosane Ushirobira.

In [46], a distributed observer was presented to estimate the state of a linear time-invariant plant in finite-time in each observer node. The design was based on a decomposition into locally observable and unobservable substates and on properties of homogeneous systems. Each observer node can reconstruct in finite-time its locally observable substate with its measurements only. Then exploiting the coupling, a finite-time converging observer was constructed for the remaining states by adding the consensus terms.

7.10. Parameter estimation in finite-time without PE

Participant: Denis Efimov.

The problem of estimation in the linear regression model was studied in [24], [48], [25] under the hypothesis that the regressor may be excited on a limited initial interval of time only. Then the estimation solution was searched on a finite interval of time also based on the framework of finite-time or fixed-time converging dynamical systems. The robustness issue was analyzed and a short-time input-to-state stability property was introduced for fixed-time converging time-varying systems with a sufficient condition, which was formulated with the use of a Lyapunov function. Several estimation algorithms were proposed and compared with existing solutions.

7.11. Quadrotor control

Participant: Andrey Polyakov.

The problem of a state feedback design for control of a quadrotor system under state and time constraints was studied in [49]. Convex embedding approach and Implicit Lyapunov function were employed to design a finite-time controller. The feedback gains were calculated by a system of LMIs (see video of experiments).

7.12. Blimp robot control

Participant: Denis Efimov.

The papers [50], [26] presented the robust controller design for an indoor blimp robot to achieve application such as the surveillance. The commonly used 6 degrees of freedom dynamic model was simplified under reasonable assumptions and decoupled into two independent parts. The blimp simplified horizontal plane movement model was complemented with disturbance terms to ensure the modeling accuracy, then it was transformed to a simpler form for the ease of controller design. Next, the disturbance terms were evaluated by the designed real-time estimator, and the perturbation estimates were compensated in the conceived motion controller for cancellation of the influence of disturbances. The performance and robustness of the disturbance compensation-based controller were verified by both simulations and experiments on the developed blimp robot.

7.13. Output finite-time stability and stabilization

Participants: Denis Efimov, Andrey Polyakov.

The equivalent Lyapunov characterizations of output finite-time stability were presented in [51]. Another sufficient condition for output finite-time stability was presented in [52]. Based on this condition a scheme of adaptive finite-time control design was provided. The presented results were obtained with the use of homogeneity property.

BONUS Project-Team

7. New Results

7.1. Decomposition-based optimization

During the year 2019, we have investigated decomposition-based optimization in the decision space as well as in the objective space. In the decision space, we have considered discrete as well as continuous problems. For discrete problems, we have reinvestigated our interval-based decomposition approach proposed in [7] as a baseline to explore ultra-scale Branch-and-Bound algorithms using Chapel [13]. The contribution is presented in Section 7.3 . For continuous problems, we have extended the geometric fractal decomposition-based approach [10] to multi-objective optimization [32] and importantly to parallel computing [17] to deal with scalability, one of the major scientific challenges as pointed out in Section 3.1 . In the objective space, we have deeply studied in [23] the surrogate-assisted multi-objective optimization based on decomposition. The contributions are summarized in the following.

7.1.1. Parallel fractal decomposition for big continuous optimization problems

Participants: El-Ghazali Talbi [contact person], Amir Nakib [Laboratoire Images, Signaux et Systèmes Intelligents (LISSI), Paris], Léo Souquet [Laboratoire Images, Signaux et Systèmes Intelligents (LISSI), Paris].

Fractal Decomposition Algorithm (FDA) is a metaheuristic that was recently proposed to solve high dimensional continuous optimization problems [10]. This approach is based on a geometric fractal decomposition which divides the search space while looking for the optimal solution. While FDA and its fractal decomposition has shown to be an effective optimization algorithm, its running time grows significantly as the problems dimension increases. To deal with this expensive computational time, a parallelized version of FDA, called Parallel Fractal Decomposition Algorithm (PFDA) is proposed in [17]. The focus is on parallelizing the exploration and exploitation phases of the original algorithm in a multi-threaded environment. The performances of PFDA are evaluated on the same Benchmark used to illustrate FDA efficiency, the SOCO 2011. It is composed of 19 functions with *dimensions going from 50 to 5000*. The results show that PFDA allows one to achieve similar performances as the original version with a significantly reduced computational time.

7.1.2. Deterministic multi-objective fractal decomposition

Participants: El-Ghazali Talbi [contact person], Amir Nakib [Laboratoire Images, Signaux et Systèmes Intelligents (LISSI), Paris], Léo Souquet [Laboratoire Images, Signaux et Systèmes Intelligents (LISSI), Paris].

We have proposed in [32] a new deterministic Multi-objective Fractal Decomposition Algorithm (Mo-FDA). The original FDA [10] was designed for single-objective large-scale continuous optimization problems. It is based on a "divide-and-conquer" strategy and a geometric fractal decomposition of the search space using hyperspheres. In this work, a scalarization approach is used to deal with multi-objective problems. The performance of Mo-FDA is compared to state-of-the-art algorithms from the literature on classical benchmarks of multi-objective optimization.

7.1.3. Surrogate-assisted multi-objective optimization based on decomposition

Participants: Nicolas Berveglieri, Bilel Derbel, Arnaud Liefooghe, Hernan Aguirre [Shinshu University, Japan], Kiyoshi Tanaka [Shinshu University, Japan].

A number of surrogate-assisted evolutionary algorithms are being developed for tackling expensive multi-objective optimization problems. On the one hand, a relatively broad range of techniques from both machine learning and multi-objective optimization can be combined for this purpose. Different taxonomies exist in order to better delimit the design choices, advantages and drawbacks of existing approaches. On the other hand, assessing the relative performance of a given approach is a difficult task, since it depends on the characteristics of the problem at hand. In [23], we focus on surrogate-assisted approaches using objective space decomposition as a core component. We propose a refined and fine-grained classification, ranging from EGO-like approaches to filtering or pre-screening. More importantly, we provide a comprehensive comparative study of a representative selection of state-of-the-art methods, together with simple baseline algorithms. We rely on selected benchmark functions taken from the bbob-biobj benchmarking test suite, that provides a variable range of objective function difficulties. Our empirical analysis highlights the effect of the available budget on the relative performance of each approach, and the impact of the training set and of the machine learning model construction on both solution quality and runtime efficiency.

7.2. ML-assisted optimization

As pointed out in our research program 3.2 , we investigate the ML-assisted optimization following two directions: building efficiently surrogates to deal with expensive black-box objective functions and automatically building and predicting/improving the performance of metaheuristics through landscape/problem structure analysis. Regarding surrogate-assisted optimization, we put the focus in [31] on mixed discrete-continuous optmization problems, one of the major challenges of this topic. In addition, we focused on the evolution control and batch parallelism to deal with another challenge which consists in efficiently integrating surrogate models (Bayesian neural networks in this case) in evolutionary algorithms [FGCS-Briffoteaux, à compléter]. From the application point of view, we applied our approaches to three different real-world simulation-based problems in the context of three collaborations: multi-stage optimal scheduling of virtual power plants (collaboration with electrical engineering department of UMONS University, Belgium) in [27], aerospace vehicle design (collaboration with ONERA, Paris) in [31], and resource allocation for the Tuberculosis edidemic control (Monash University) in [FGCS-Briffoteax, à compléter]. The two latter ones are summarized in the following sections. Regarding the second direction, we thoroughly study in [16] the impact of landscape characteristics on the performance of search heuristics for black-box multi-objective combinatorial optimization problems. We also introduce in [26] new insightful features for continuous exploratory landscape analysis and algorithm selection. In addition, as pointed out in 3.2 , variable selection is highly important to deal with BOPs. In [28], in collaboration with our partners from Shinshu University we come out with an efficient method to classify variables influencing convergence and increase their recombination rate. The contributions are summarized in the following.

7.2.1. Surrogate-assisted optimization of constrained mixed variable problems: application to the design of a launch vehiclethrust frame.

Participants: El-Ghazali Talbi [contact person], Julien Pelamatti, Loïc Brevault [ONERA], Mathieu Balesdent [ONERA], Yannick Guerin [CNES].

Within the framework of complex systems design, such as launch vehicles, numerical optimization is an essential tool as it allows to reduce the design process time and costs. The inclusion of discrete variables in the design process allows to extend the applicability of numerical optimization methods to a broader number of systems and sub-systems. In [31], a recently proposed adaptation of the Efficient Global Optimization method (EGO) for constrained mixed-variable problems is applied to the design optimization of a launch vehicle thrust frame, which depends on both continuous sizing parameters and discrete variables characterizing the number of structural reinforcements. The EGO adaptation that is considered is based on a redefinition of the Gaussian Process kernel as a product between a standard continuous kernel and a second kernel representing the covariance between the discrete variable values. From the results obtained on an analytical test-case as well as on the launch vehicle thrust frame design optimization, it is shown that the use of the mixed-variable EGO algorithm allows to converge towards the neighborhoods of the problems optima with fewer function evaluations when compared to reference optimization algorithms.

7.2.2. Parallel Batched Bayesian Neural Network-assisted GA versus q-EGO

Participants: Guillaume Briffoteaux, Maxime Gobert, Jan Gmys, Nouredine Melab [contact person], Romain Ragonnet [School of Public Health and Preventive Medicine, Monash University, Australia], Mohand Mezmaz [University of Mons, Blegium], Daniel Tuyttens [University of Mons, Blegium].

Surrogate-based optimization has been widely used to deal with expensive black-box simulation-based objective functions. The use of a surrogate model allows to reduce the number of calls to the costly simulator. In (SWEVO, Briffoteaux et al., 2020), the Efficient Global Optimization (EGO) reference framework is challenged by a Bayesian Neural Network-assisted Genetic Algorithm, namely BNN-GA. The Bayesian Neural Network (BNN) surrogate provides an uncertainty measure of the prediction that allows to compute the Expected Improvement of a candidate solution in order to improve the exploration of the objective space. BNN is also more reliable than Kriging models for high-dimensional problems and faster to set up thanks to its incremental training. In addition, we propose a batch-based approach for the parallelization of BNN-GA that is challenged by a parallel version of EGO, called q-EGO. Parallel computing is a complementary way to deal with the computational burden of simulation-based optimization. The comparison of the two parallel approaches is experimentally performed through several benchmark functions and two real-world problems within the scope of Tuberculosis Transmission Control (TBTC). The results demonstrate the efficiency and scalability of the parallel batched BNN-GA for small budgets, outperforming it for larger budgets on the benchmark testbed. A significant improvement of the solutions is obtained for two TBTC problems. Finally, our study proves that parallel batched BNN-GA is a viable alternative to q-EGO approaches being more suitable for high-dimensional problems and parallelization impact.

7.2.3. Landscape-aware performance prediction and algorithm selection for single- and multi-objective evolutionary optimization

Participants: Arnaud Liefooghe, Bilel Derbel, Fabio Daolio [ASOS.com, UK], Sébastien Verel [LISIC, Université du Littoral Côte d'Opale], Hernan Aguirre [Shinshu University, Japan], Kiyoshi Tanaka [Shinshu University, Japan].

Extracting a priori knowledge informing about the landscape underlying an unknown optimization problem has been proved extremely useful for different purposes, such as designing finely-tuned algorithms, predicting algorithm performance and designing automated portfolio-based solving approaches. Considering black-box continuous single-objective optimization problems, in [26], we adopt an exploratory landscape analysis approach providing a unified methodology for integrating landscape features into sophisticated machine learning techniques. More precisely, we consider the design of novel informative and cheap landscape features on the basis of the search tree constructed by the so-called SOO (Simultaneous Optimistic Optimization) algorithm, which is arguably a global optimizer coming from the machine learning community and having its foundations in the multi-armed bandit theory. We thereby provide empirical evidence on the accuracy of the proposed features for both predicting high-level problem properties, and tackling the algorithm selection problem with respect to a given portfolio of available solvers and a broad range of optimisation problems taking from the specialized literature and exposing different degrees of difficulty.

Considering black-box combinatorial multi-objective optimization problems, in [16], we expose and contrast the impact of landscape characteristics on the performance of search heuristics for black-box multi-objective combinatorial optimization problems. A sound and concise summary of features characterizing the structure of an arbitrary problem instance is identified and related to the expected performance of global and local dominance-based multi-objective optimization algorithms. We provide a critical review of existing features tailored to multi-objective combinatorial optimization problems, and we propose additional ones that do not require any global knowledge from the landscape, making them suitable for large-size problem instances. Their intercorrelation and their association with algorithm performance are also analyzed. This allows us to assess the individual and the joint effect of problem features on algorithm performance, and to highlight the main difficulties encountered by such search heuristics. By providing effective tools for multi-objective landscape analysis, we highlight that multiple features are required to capture problem difficulty, and we provide further insights into the importance of ruggedness and multimodality to characterize multi-objective combinatorial landscapes.

7.2.4. Estimating Relevance of Variables for Effective Recombination

Participants: Arnaud Liefooghe, Bilel Derbel, Sébastien Verel [LISIC, Université du Littoral Côte d'Opale], Taishi Ito [Shinshu University, Japan], Hernan Aguirre [Shinshu University, Japan], Kiyoshi Tanaka [Shinshu University, Japan].

Dominance and its extensions, decomposition, and indicator functions are well-known approaches used to design MOEAs. Algorithms based on these approaches have mostly sought to enhance parent selection and survival selection. In addition, several variation operators have been developed for MOEAs. In [28], we focus on the classification and selection of variables to improve the effectiveness of solution search. We propose a method to classify variables that influence convergence and increase their recombination rate, aiming to improve convergence of the approximation found by the algorithm. We incorporate the proposed method into NSGA-II and study its effectiveness using three-objective DTLZ and WFG benchmark functions, including unimodal, multimodal, separable, non-separable, unbiased, and biased functions. We also test the effectiveness of the proposed method on a real-world bi-objective problem. Simulation results verify that the proposed method can contribute to achieving faster and better convergence in several kinds of problems, including the real-world problem.

7.3. Towards ultra-scale Big Optimization

During the year 2019, we have addressed the ultra-scale optimization research line following two main directions: designing efficient optimization algorithms dealing with scalability in terms of number of processing cores and/or in terms of the size of tackled problem instances. For the first direction, the challenge is to take into account in addition to the traditional performance objective the productivity awareness which is highly important to deal with the increasing complexity of medern supercomputers. With the short-term perspective of establishing a collaboration with one of the major HPC builders (Cray Inc.), we have investigated in [13], [24], [25] the exascale-aware Chapel language. Regarding the second direction, we contributed to solve difficult unsolved flow-shop [15] and Quadratic Assignement Problem (QAP) [22] permutation problem instances using moderate-scale parallelism. The contributions are summarized in the following.

7.3.1. Towards ultra-scale Branch-and-Bound using a high-productivity language

Participants: Tiago Carneiro Pessoa, Jan Gmys, Nouredine Melab, Daniel Tuyttens [University of Mons, Blegium].

Productivity is crucial for designing ultra-scale algorithms able to harness modern supercomputers which are increasingly complex, including millions of processing cores and heterogeneous building-block devices. In [13], we investigate the partitioned global address space (PGAS)-based approach using Chapel for the productivity-aware design and implementation of distributed Branc-and-Bound (B&B) for solving large optmization problems. The proposed algorithms are intensively experimented using the Flow-shop scheduling problem as a test-case. The Chapel-based implementation is compared to its MPI+X-based traditionally used counterpart in terms of performance, scalability, and productivity. The results show that Chapel is much more expressive and up to $7.8\times$ more productive than MPI+Pthreads. In addition, the Chapel-based search presents performance equivalent to MPI+Pthreads for its best results on 1024 cores and reaches up to 84% of the linear speedup. However, there are cases where the built-in load balancing provided by Chapel cannot produce regular load among computer nodes. In such cases, the MPI-based search can be up to $4.2\times$ faster and reaches speedups up to $3\times$ higher than its Chapel-based counterpart. Thorough feedback on the experience is given, pointing out the strengths and limitations of the two opposite approaches (Chapel vs. MPI+X). To the best of our knowledge, the present study is pioneering within the context of exact parallel optimization.

7.3.2. A computationally efficient Branch-and-Bound algorithm for the permutation flow-shop scheduling problem

Participants: Jan Gmys, Nouredine Melab, Mohand Mezmaz [University of Mons, Blegium], Daniel Tuyttens [University of Mons, Blegium].

In [15], we propose an efficient Branch-and-Bound (B&B) algorithm for the permutation flow-shop problem (PFSP) with makespan objective. We present a new node decomposition scheme that combines dynamic branching and lower bound refinement strategies in a computationally efficient way. To alleviate the computational burden of the two-machine bound used in the refinement stage, we propose an online learning-inspired mechanism to predict promising couples of bottleneck machines. The algorithm offers multiple choices for branching and bounding operators and can explore the search tree either sequentially or in parallel on multicore CPUs. In order to empirically determine the most efficient combination of these components, a series of computational experiments with 600 benchmark instances is performed. A main insight is that the problem size, as well as interactions between branching and bounding operators substantially modify the trade-off between the computational requirements of a lower bound and the achieved tree size reduction. Moreover, we demonstrate that parallel tree search is a key ingredient for the resolution of large problem instances, a strong super-linear speedups can be observed. An overall evaluation using two well-known benchmarks indicates that the proposed approach is superior to previously published B&B algorithms. For the first benchmark we report the exact resolution – within less than 20 minutes – of two instances defined by 500 jobs and 20 machines that remained open for more than 25 years, and for the second a total of 89 improved best-known upper bounds, including proofs of optimality for 74 of them.

7.3.3. A Parallel Tabu Search for the Large-scale Quadratic Assignment Problem

Participants: Omar Abdelkafi, Bilel Derbel, Arnaud Liefooghe.

Parallelization is an important paradigm for solving massive optimization problems. Understanding how to fully benefit form the aggregated computing power and what makes a parallel strategy successful is a difficult issue. In [22], we propose a simple parallel iterative tabu search (PITS) and study its effectiveness with respect to different experimental settings. Using the quadratic assignment problem (QAP) as a case study, we first consider different small-and medium-size instances from the literature and then tackle a large-size instance that was rarely considered due the its inherent solving difficulty. In particular, we show that a balance between the number of function evaluations each parallel process is allowed to perform before resuming the search is a critical issue to obtain an improved quality.

CELESTE Project-Team

6. New Results

6.1. Minimal penalty algorithms for model selection

Birgé and Massart proposed in 2001 the slope heuristics as a way to choose optimally from data an unknown multiplicative constant in front of a penalty. It is built upon the notion of minimal penalty, and it has been generalized since to some "minimal-penalty algorithms". The survey [3] by S. Arlot reviews the theoretical results obtained for such algorithms, with a self-contained proof in the simplest framework, precise proof ideas for further generalizations, and a few new results. Explicit connections are made with residual-variance estimators —with an original contribution on this topic, showing that for this task the slope heuristics performs almost as well as a residual-based estimator with the best model choice— and some classical algorithms such as L-curve or elbow heuristics, Mallows' C_p, and Akaike's FPE. Practical issues are also addressed, including two new practical definitions of minimal-penalty algorithms that are compared on synthetic data to previously-proposed definitions. Finally, several conjectures and open problems are suggested as future research directions. This extensive survey is followed by a discussion by 13 authors, and a rejoinder in which another original result is proved (theoretical validation of the slope heuristics when all models in the collection are biased).

6.2. Kernel change-point detection

In collaboration with A. Celisse and Z. Harchaoui, S. Arlot worked on the change-point problem with data belonging to a general set. They built a penalty for choosing the number of change-points in the kernel-based method of Harchaoui and Cappé (2007). This penalty generalizes the one proposed by Lebarbier (2005) for one-dimensional signals. They prove in [4] a non-asymptotic oracle inequality for the proposed method, thanks to a new concentration result for some function of Hilbert-space valued random variables. Experiments on synthetic and real data illustrate the accuracy of our method, showing that it can detect changes in the whole distribution of data, even when the mean and variance are constant. This method has since been used successfully by several authors in various applied contexts.

6.3. A probabilistic method to characterize genomic alterations of tumors

Characterizing the genomic copy number alterations (CNA) in cancer is of major importance in order to develop personalized medicine. Single nucleotide polymorphism (SNP) arrays are still in use to measure CNA profiles. Among the methods for SNP-array analysis, the Genome Alteration Print (GAP) by Popova et al, based on a preliminary segmentation of SNP-array profiles, uses a deterministic approach to infer the absolute copy numbers profile. C. Keribin with Y. Liu, Y. Rozenholch and T. Popova developed a probabilistic model in [9] for GAP and define a Gaussian mixture model where centers are constrained to belong to a frame depending on unknown parameters such as the proportion of normal tissue. The estimation is performed using an expectation-maximization (EM) algorithm to recover the parameters characterizing the genomic alterations as well as the most probable copy number change of each segment and the unknown proportion of normal tissue. The tumor ploidy can be deduced from penalized model selection criterion. The model is tested on simulated and real data.

Surprisingly, the BIC selection criterion cannot recover the actual ploidy in the real data sets as slope heuristics do, even though all models are wrong. C. Keribin, in a discussion of S. Arlot's survey, gave some arguments to explain these behaviors [8].

6.4. New results for stochastic bandits

M. Brégère and G. Stoltz, in collaboration with P. Gaillard (Sierra team) and Y. Goude (EDF), provided a methodology in [5] based on a modeling by linear bandits, for managing (influencing) electricity consumption by sending tariff incentives. The main result is the very modeling of the problem: consumption is modeled as a generalized additive model based on the probabilistic allocation of tariffs picked and on the context (given by the type of day, hour of the day, weather conditions, etc.). Mathematical results are, on the other hand, direct extensions of earlier results for the LinUCB algorithm (see Li et al., 2010; Chu et al., 2011; Abbasi-Yadkori et al., 2011). Simulations on realistic data are provided: for bandit algorithms, one needs a data simulator, which we created based on an open data set consisting of households in London.

A second important result was obtained by H. Hadiji: he characterized the cost of adaptation to the unknown (Höderian) smoothness payoff functions in continuum-armed bandits [14]. He first rewrote and slightly extended the regret lower bounds exhibited by Locatelli and Carpentier (2018), and then exhibited an algorithm with matching regret upper bounds. This algorithm, unlike virtually all previous algorithms in X-armed bandits, which zoomed in as time passes, zooms out as time passes. This solves a problem that had been open for several years.

Also, H. Hadiji and G. Stoltz, in collaboration with P. Ménard (SequeL team) and A. Garivier, submitted a revised version of their results of simultaneous optimality (from both a distribution-dependent and a distribution-free viewpoints) for a variant of the KL-UCB algorithm in the case of vanilla K-armed stochastic bandits [22].

6.5. Robust risk minimization for machine learning

In collaboration with S. Minsker (USC), T. Mathieu worked on obtaining new excess risk bounds in robust empirical risk minimization. The method proposed in [29] is inspired from the robust risk minimization procedure using median-of-means estimators in Lecué, Lerasle and Mathieu (2018). The obtained excess risk are faster than the so-called "slow rate of convergence" obtained for the minimization procedure in Lecué, Lerasle and Mathieu (2018) and a slightly modified procedure achieves a minimax rate of convergence under low moment assumptions. Experiments on synthetic corrupted data and real dataset illustrate the accuracy of the method showing high performance in classification and regression tasks in a corrupted setting.

6.6. Optimal pair-matching

The sequential pair-matching problem appears in many applications (in particular for the internet) where one wants to discover, sequentially, good matches between pairs of individuals, for a given budget. C. Giraud, Y. Issartel, L. Lehéricy and M. Lerasle propose a formulation of this problem as a special bandit problem on graphs [23]. Formally, the set of individuals is represented by the nodes of a graph where the edges, unobserved at first, represent the potential good matches. The algorithm queries pairs of nodes and observes the presence/absence of edges. Its goal is to discover as many edges as possible with a fixed budget of queries. Pair-matching is a particular instance of multi-armed bandit problem in which the arms are pairs of individuals and the rewards are edges linking these pairs. This bandit problem is non-standard though, as each arm can only be played once.

Given this last constraint, sublinear regret can be expected only if the graph has some underlying structure. C. Giraud, Y. Issartel, L. Lehéricy and M. Lerasle show in [23] that sublinear regret is achievable in the case where the graph is generated according to a Stochastic Block Model (SBM) with two communities. Optimal regret bounds are computed for this pair-matching problem. They exhibit a phase transition related to the Kesten-Stigund threshold for community detection in SBMs. In practice, it is meaningful to constrain each node to be sampled less than a given amount of times, in order to avoid concentration of queries on a set of individuals. This setting is more challenging both on the statistical side and the algorithmic side. Optimal rates are also derived in this context, exhibiting how the regret deteriorates with this constraint.

6.7. Minimax estimation of network complexity in graphon model

In network analysis, the graphon model has attracted a lot of attention as a non-parametric model with some universal properties. However, this approach suffers from interpretability and identifiability issues in practice. A first solution to this problem was obtained by Y. Issartel: he introduces an identifiable and interpretable functional of the graphon, which measures the complexity of network [25]. It has simple interpretations on popular examples of random graphs: it matches the number of communities in stochastic block models; the dimension of the Euclidean space in random geometric graphs; the regularity of the link function in Hölder graphons. He also provides an estimation procedure of this complexity that is minimax optimal.

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 2Hz 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 random 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.

Publications: Frontiers in Physiology, Frontiers, 2019, 10, pp.480 (1-18), HAL

Second international Summer Institute on Network Physiology, Jul 2019 HAL

7.2. Differential diagnosis between atypical Parkinsonian syndromes

Participants: B. Das , K. Daoudi , J. Kemplir , J. Rusz .

In the early stage of disease, the symptoms of Parkinson's disease (PD) are similar to atypical Parkinsonian syndromes (APS). The early differential diagnosis between PD and APS and within APS is thus a very challenging task. It turns out that speech disorder is an early and common symptom to PD and APS. The goal of research is to develop a digital marker based on speech analysis in order to assist the neurologists in their diagnosis. We addressed the problem of differential diagnosis between two APS, Progressive Supranuclear Palsy (PSP) and Multiple System Atrophy (MSA). Using linear discriminant analysis we designed an hypokinetic and an ataxic dysarthria measure which yield a discrimination between PSP and MSA with a high accuracy (88%). This result indicates that hypokinetic and ataxic dysarthria convey valuable discriminative information when mutually considered.

Publication: ICASSP 2019 HAL

7.3. Turbulent dynamics of ocean upwelling

Participants: A. El Aouni , V. Garçon , J. Sudre , H. Yahia , K. Daoudi , K. Minaoui .

The region along the NorthWest African coast (20° N to 36° N and 4° W to 19° W) is characterized by a persistent and variable upwelling phenomenon almost all year round. In this article, the upwelling features are investigated using an algorithm dedicated to delimit the upwelling area from thermal and biological satellite observations. This method has been developed specifically for sea-surface temperature (SST) images, since they present a high latitudinal variation, which is not present in chlorophyll-a concentration images. Developing on the proposed approach, the spatial and temporal variations of the main physical and biological upwelling patterns are studied. Moreover, a study on the upwelling dynamics, which explores the interplay between the upwelling spatiotemporal extents and intensity, is presented, based on a 14-year time archive of weekly SST and chlorophyll-a concentration data.

Publication: IEEE Transactions on Geoscience and Remote Sensing, HAL

7.4. Fourier approach to Lagrangian vortex detection

Participants: A. El Aouni , H. Yahia , K. Daoudi , K. Minaoui .

We study the transport properties of coherent vortices over a finite time duration. Here we reveal that such vortices can be identified based on frequency-domain representation of Lagrangian trajectories. We use Fourier analysis to convert particles' trajectories from their time domain to a presentation in the frequency domain. We then identify and extract coherent vortices as material surfaces along which particles' trajectories share similar frequencies. Our method identifies all coherent vortices in an automatic manner, showing high vortices' monitoring capacity. We illustrate our new method by identifying and extracting Lagrangian coherent vortices in different two-and three-dimensional flows.

Publication: Chaos, American Institute of Physics, HAL

7.5. Surface mixing and biological activity

Participants: A. El Aouni , K. Daoudi , H. Yahia , K. Minaoui , A. Benazzouz .

Near-shore water along the NorthWest African margin is one of the world's major upwelling regions. It is associated with physical structures of oceanic fronts which influence the biological productivity. The study of these coherent structures in connection with chlorophyll concentration data is of fundamental importance for understanding the spatial distributions of the plankton. In this work, we study the horizontal stirring and mixing in different upwelling areas using Lagrangian coherent structures (LCSs). These LCSs are calculated using the recent geodesic theory of LCSs. We use these LCSs to study the link between the chlorophyll fronts concentrations and surface mixing, based on 10 years of satellite data. These LCSs move with the flow as material lines, thus the horizontal mixing is calculated from the intersection of these LCSs with the finite time Lyapunov exponents (FTLEs) maps. We compare our results with those of a recent study conducted over the same area, but based on Finite Size Lyapunov Exponents (FSLEs) whose output is a plot of scalar distributions. We discuss the differences between FSLE and geodesic theory of LCS. The latter yields analytical solutions of LCSs, while FSLEs can only provide LCSs for sharp enough ridges of nearly constant height.

Publication: Chaos, American Institute of Physics, HAL

7.6. Contribution and influence of coherent mesoscale eddies off the North-West African upwelling on the open ocean

Participants: A. El Aouni , K. Daoudi , H. Yahia , K. Minaoui .

Eastern Boundary Upwelling zones include some of the most productive ecosystems in the world, particularly the NorthWest (NW) African upwelling which presents one of the world's major upwelling regions. This latter is forced by the equator-ward trade winds which are known to exhibit mesoscale instabilities; thus, in addition to upwelled cold and nutrient-rich deep waters, significant energy is transferred into mesoscale fronts and eddies in the upper ocean. Oceanic structures of type eddies are well know to stir and mix surrounding water masses. However, they can also carry and transport organic matter and marine in a coherent manner. Here, we are interested in those that remain coherent. The Aim of this work, is to understand the impact and the contribution of the mesoscale eddies off the NW African margin on the open ocean. Our approach to analyze such coherent eddies is based upon the use of our recently developed technique from nonlinear dynamics theory, which is capable of identifying coherent vortices and their centers in an automatic manner. The role of these mesoscale eddies is investigated based on a statistical study of eddies properties off NW African margin (cyclone/anticyclone, their lifetimes, traveled distance, translational speeds, quantity of water masses transported to the open ocean...). This statistical study is carried out over a sets of 24 years (spans from January 1993 to December 2016) of sea surface velocity field derived from satellite surface altimetry under the geostrophic approximation.

Publication: SIAM Conference on Mathematics of Planet Earth, (MPE18) HAL

7.7. Defining coherent vortices from particles trajectories

Participants: A. El Aouni , H. Yahia , K. Daoudi , K. Minaoui .

Tracer patterns in the ocean, such as sea surface temperature, chlorophyll concentration and salinity suggest the emergence of coherence even in the ocean, typically with fluxes dominated by advective transport over diffusion. Mesoscale eddies are known to govern advective transport in the ocean, with typical horizontal scales $\mathcal{O}(100km)$ and timescales of $\mathcal{O}(weeks)$. These oceanic structures are omnipresent in the ocean and usually exhibit different properties to their surroundings. They are known to stir and mix surroundings water masses as well as by their ability to trap and carry fluid properties in a coherent manner. As the effect of these mesoscale eddies on the global circulation is remarkable, we focused on studying and understanding the dynamic transport properties of these coherent oceanic structures. For this reason, we have developed a Lagrangian method to identify and extract Lagrangian coherent vortices. The method analyzes particles' trajectories to identify vortices' boundaries and their attractor centers. Indeed, it is based on a decomposition of particle trajectory into two parts: closed curves which give information about uniformly rotating flow, and one that describes the mean displacement. The former part yields an objective measure of material rotation. We define Lagrangian coherent vortex as closed material lines in which fluid parcels complete the same polar rotation. This turns out to be filled with outward-increasing closed contours of the Lagrangian Averaged Closed Curve Length.

Publications: 3 articles submitted.

7.8. Soft hydrogel particle packings

Participants: J. Bares , N. Brodu , H. Zheng , J. A. Dijksman .

We provide the raw data from several years worth of effort on index matching experiments on soft hydrogel particle packings exposed to various loading conditions. Many of the data sets have not before been used, described explicitly in scientific publications or even analyzed. We will present a general overview of methods used to perform the imaging experiments. We provide particle-level information extracted from the 3D images, including contact forces and particle shapes, along with complementary boundary force measurements. We also provide a final working version of the code used to extract these microscopic features.

Publication: *Releasing data from mechanical tests on three dimensional hydrogel sphere packings*, Granular Matter, HAL

7.9. Feature based reconstruction model for fluorescence microscopy image denoising

Participants: S. K. Maji , H. Yahia .

: the advent of Fluorescence Microscopy over the last few years have dramatically improved the problem of visualization and tracking of specific cellular objects for biological inference. But like any other imaging system, fluorescence microscopy has its own limitations. The resultant images suffer from the effect of noise due to both signal dependent and signal independent factors, thereby limiting the possibility of biological inferencing. Denoising is a class of image processing algorithms that aim to remove noise from acquired images and has gained wide attention in the field of fluorescence microscopy image restoration. In this paper, we propose an image denoising algorithm based on the concept of feature extraction through multifractal decomposition and then estimate a noise free image from the gradients restricted to these features. Experimental results over simulated and real fluorescence microscopy data prove the merit of the proposed approach, both visually and quantitatively.

Publication: Scientific Reports, Nature Publishing Group, HAL

7.10. InnovationLab with I2S, sparse signals & optimisation

Participants: M. Martin, H. Yahia, A. Zebadua, S. Sakka, N. Brodu, K. Daoudi, A. Cherif [I2S], J. L. Vallancogne [I2S], A. Cailly [I2S], A. Billy [I2S], B. Lebouill [I2S].

During 2019:

Linear inverse problems in image processing, denoising, deconvolution, non-convex optimization, plug, and play algorithms.

HDR (High Dynamic Range) : C++ implementation with OpenCV library; code deposited on gitlab, sharing with I2S company, enhancement of the code architecture. GPU implementation.

Reflecting improvement: development and C++ implementation.

3D reconstruction: implementation and test with openMVG and openMVS libraries. Depth map enhancement through non-convex optimization.

Image smoothing implementation [57].

CPU and GPU patchmatch implementation [55].

INOCS Project-Team

7. New Results

7.1. Large scale complex structure optimization

Joint order batching and picker routing problem: Order picking is the process of retrieving products from 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 [64]. Moreover, we propose 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 generally 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 and take into account in the development of an efficient subroutine, called oracle. We therefore investigate whether such an oracle allows for an effective exponential formulation. 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. Finally, this approach is also applied to the HappyChic industrial case to demonstrate its interest for this field of application [67], [45].

Logistics network design problem: Planning transportation operations within a supply chain is a difficult task that is often outsourced to logistics providers, in practice. At the tactical level, the problem of distributing products through a multi-echelon network is defined in the literature as the Logistics Service Network Design Problem (LSNDP). We study a LSNDP variant inspired by the management of restaurant supply chains. In this problem, a third party carrier seeks to cost-effectively source and fulfill customer demands of products through a tri-echelon supply chain composed of suppliers, warehouses, and customers. We propose an exact solution method based on partial Benders decompositions, where the master problem is strengthened by the addition of aggregated information derived from the subproblem. More specifically, we introduce a high-level dynamic Benders approach where the aggregated information used to strengthen the master is refined iteratively. In an extensive computational study, we demonstrate that our dynamic Benders strategy produces provably high-quality solutions and we validate the interest of refining the master problem in the course of a partial Benders decomposition-based scheme [72].

Multi commodity vehicle routing problem: We study vehicle routing problems considering multiple commodities, with applications in the local fresh food supply chains. The studied supply chain contains two echelons with three sets of actors: suppliers, distribution centers and customers. Suppliers are farmers that produce some fresh foods. Distribution centers are in charge of consolidation and delivery of the products to customers. Distribution centers collect products from the suppliers that perform direct trips. Products are delivered to the customers with a fleet of vehicles performing routes. Each customer requires several commodities, and the farmers produce a limited quantity of these commodities. For the minimization of the transportation cost, it is beneficial that a single customer is delivered by several vehicles. However, for the convenience of the customer, it is imposed that a single commodity is delivered at once by a single vehicle. Hence, different commodities have been explicitly considered. The complete problem is named Multi-Commodity two-echelon Distribution Problem (MC2DP). The restricted problem that addresses only the delivery from a single distribution center is named Commodity constrained Split Delivery Vehicle Routing Problem (C-SDVRP). We first propose a heuristic based on the Adaptive Large Neighborhood Search (ALNS) for the C-SDVRP [22]. Then, we address the whole problem (MC2DP) with collection and delivery operations and multiple distribution centers. In order to tackle this complex problem, we propose to decompose the problem: collection and delivery are sequentially solved [53], [54].

Generalized routing problems: We study routing problems that arise in the context of last mile delivery when multiple delivery options are proposed to the customers. The most common option to deliver packages is home/workplace delivery. Besides, the delivery can be made to pick-up points such as dedicated lockers or stores. In recent years, a new concept called trunk/in-car delivery has been proposed. Here, customers' packages can be delivered to the trunks of cars. Our goal is to model and develop efficient solution approaches for routing problems in this context, in which each customer can have multiple shipping locations. First, we study the single-vehicle case in the considered context, which is modeled as a Generalized Traveling Salesman Problem with Time Windows (GTSPTW). Four mixed integer linear programming formulations and an efficient branch-and-cut algorithm are proposed. Then, we study the multi-vehicle case which is denoted Generalized Vehicle Routing Problem with Time Windows (GVRPTW). An efficient column generation based heuristic is proposed to solve it [60], [61], [59], [37].

Joint management of demand and offer 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. This growing in 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. We have proposed an optimization problem aiming jointly to manage the offer and the demand. More precisely, discrete choice models representing the choices made by couriers and customers are integrated into the same optimization model. The originality of the contribution is based on the integration of variables of different natures in the same model and the development of integrated resolution methods. On the basis of a closed form of discrete choice models, we have reformulated the problem as a non-linear optimization problem. The resolution of this model by classical solvers requires coupling exact methods with heuristics in order to define a first initial solution [47], [58].

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 [21].

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 (1) aligning sequence reads from a set of individual(s) with respect to a reference genome and (2) 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 [29] 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 a graph 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 [75].

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 [24].

7.2. Bilevel Programming

Pricing for 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 (Léonard Von Niederhausern PhD thesis [76]). 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 modeled 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 [13], [76].

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 [38], [46].

Linear bilevel optimization: One of the most frequently used approaches to solve linear bilevel optimization problems consists in replacing the lower-level problem with its Karush–Kuhn–Tucker (KKT) conditions and by reformulating the KKT complementarity conditions using techniques from mixed-integer linear optimization. The latter step requires to determine some big-M constant in order to bound the lower level's dual feasible set such that no bilevel-optimal solution is cut off. In practice, heuristics are often used to find a big-M although it is known that these approaches may fail. In [69], we consider the hardness of two proxies for the above mentioned concept of a bilevel-correct big-M. First, we prove that verifying that a given big-M does not cut off any feasible vertex of the lower level's dual polyhedron cannot be done in polynomial time unless P = NP. Second, we show that verifying that a given big-M does not cut off any optimal point of the lower level's dual problem (for any point in the projection of the high-point relaxation onto the leader's decision space) is as hard as solving the original bilevel problem.

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 [28].

Product 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 [73].

Next in [68], we analyze a product pricing problem with single-minded customers, each interested in buying a bundle of products. The objective is to maximize the total revenue and we assume that supply is unlimited for all products. We contribute to a missing piece of literature by giving some mathematical formulations for this single-minded bundle pricing problem. We first present a mixed-integer nonlinear program with bilinear terms in the objective function and the constraints. By applying classical linearization techniques, we obtain two different mixed-integer linear programs. We then study the polyhedral structure of the linear formulations and obtain valid inequalities based on an RLT-like framework. We develop a Benders decomposition to project strong cuts from the tightest model onto the lighter models. We conclude this work with extensive numerical experiments to assess the quality of the mixed-integer linear formulations, as well as the performance of the cutting plane algorithms and the impact of the preprocessing on computation times.

Bilevel Minimum Spanning Tree Problem: Consider a graph G 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 [26].

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 [74]. 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 [23].

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 [18].

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 [15].

Third, in [39], we discuss the impact of fairness constraints in Stackelberg Security Games. Fairness constraints can be used to avoid discrimination at the moment of implementing police patrolling. We present two ways of modelling fairness constraints, one with a detailed description of the population and the other with labels. We discuss the implementability of these constraints. In the case that the constraints are not implementable we present models to retrieve pure strategies in a way that they are the closest in average to the set of fairness constraints.

Finally, in [65], we focus on Stackelberg equilibria for discounted stochastic games. We begin by formalizing the concept of Stationary Strong Stackelberg Equlibrium (SSSE) policies for such games. We provide classes of games where the SSSE exists, and we prove via counterexamples that SSSE does not exist in the general case. We define suitable dynamic programming operators whose fixed points are referred to as Fixed Point Equilibrium (FPE). We show that the FPE and SSSE coincide for a class of games with Myopic Follower Strategy. We provide numerical examples that shed light on the relationship between SSSE and FPE and the behavior of Value Iteration, Policy Iteration and Mathematical programming formulations for this problem. Finally, we present a security application to illustrate the solution concepts and the efficiency of the algorithms studied.

7.3. Robust/Stochastic programming

Locating stations in a one-way electric car sharing system under demand uncertainty: In [16], we focused 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.

Bookings in the European Gas Market: Characterisation 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 characterisation 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 [25]. Further, in [71], we show that the feasibility of a booking also can be decided in polynomial time on single-cycle networks.

Robust bilevel programs: Bilevel optimization problems embed the optimality conditions of a sub-problem into the constraints of a decision-making process. A general question of bilevel optimization occurs where the lower-level is solved (only) to near-optimality. Solving bilevel problems under limited deviations of the lower-level variables was introduced under the term "ϵ-approximation" of the pessimistic bilevel problem. In [77] the authors define special properties and a solution method for this variant in the so-called independent case, i.e., where the lower-level feasible set is independent of the upper-level decision. In [66], we generalized the approach of *Wiesemann et al. 2013*, to problems with constraints involving upper- and lower-level variables in the constraints at both levels. The purpose of this generalization is to protect the upper-level feasibility against uncertainty of near-optimal solutions of the lower-level. We call this near-optimal robustness and the generalization is a near-optimal robust bilevel problem (NORBiP). NORBiP is a bilinear bilevel problem, and this makes it very hard in general. We have defined and implemented a solution algorithm for the linear linear NORBiP [66].

MISTIS Project-Team

7. New Results

7.1. Mixture models

7.1.1. Mini-batch learning of exponential family finite mixture models

Participant: Florence Forbes.

Joint work with: Hien Nguyen, La Trobe University Melbourne Australia and Geoffrey J. McLachlan, University of Queensland, Brisbane, Australia.

Mini-batch algorithms have become increasingly popular due to the requirement for solving optimization problems, based on large-scale data sets. Using an existing online expectation-maximization (EM) algorithm framework, we demonstrate [28] how mini-batch (MB) algorithms may be constructed, and propose a scheme for the stochastic stabilization of the constructed mini-batch algorithms. Theoretical results regarding the convergence of the mini-batch EM algorithms are presented. We then demonstrate how the mini-batch framework may be applied to conduct maximum likelihood (ML) estimation of mixtures of exponential family distributions, with emphasis on ML estimation for mixtures of normal distributions. Via a simulation study, we demonstrate that the mini-batch algorithm for mixtures of normal distributions can outperform the standard EM algorithm. Further evidence of the performance of the mini-batch framework is provided via an application to the famous MNIST data set.

7.1.2. Component elimination strategies to fit mixtures of multiple scale distributions

Participants: Florence Forbes, Alexis Arnaud.

We address the issue of selecting automatically the number of components in mixture models with non-Gaussian components. As amore efficient alternative to the traditional comparison of several model scores in a range, we consider procedures based on a single run of the inference scheme. Starting from an over-fitting mixture in a Bayesian set-ting, we investigate two strategies to eliminate superfluous components.We implement these strategies for mixtures of multiple scale distributions which exhibit a variety of shapes not necessarily elliptical while remaining analytical and tractable in multiple dimensions. A Bayesian formulation and a tractable inference procedure based on variational approximation are proposed. Preliminary results on simulated and real data show promising performance in terms of model selection and computational time. This work has been presented at RSSDS 2019 - Research School on Statistics and Data Science in Melbourne, Australia [33].

7.1.3. Approximate Bayesian Inversion for high dimensional problems

Participants: Florence Forbes, Benoit Kugler.

Joint work with: Sylvain Douté from Institut de Planétologie et d'Astrophysique de Grenoble (IPAG).

The overall objective is to develop a statistical learning technique capable of solving complex inverse problems in setting with specific constraints. More specifically, the challenges are 1) the large number of observations to be inverted, 2) their large dimension, 3) the need to provide predictions for correlated parameters and 4) the need to provide a quality index (eg. uncertainty).

In the context of Bayesian inversion, one can use a regression approach, such as in the so-called Gaussian Locally Linear Mapping (GLLiM) [7], to obtain an approximation of the posterior distribution. In some cases, exploiting this approximate distribution remains challenging, for example because of its multi-modality. In this work, we investigate the possible use of Importance Sampling to build on the standard GLLiM approach by improving the approximation induced by the method and to better handle the potential existence of multiple solutions. We may also consider our approach as a way to provide an informed proposal distribution as requested by Importance Sampling techniques. We experiment our approach on simulated and real data in the context of a photometric model inversion in planetology. Preliminary results have been presented at StatLearn 2019 [76]

7.1.4. 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. . A dictionary-based learning (DBL) method was investigated to bypass inherent MRF limitations in high dimension: reconstruction time and memory requirement. The DBL method is a 3-step procedure: (1) a quasi-random sampling strategy to produce the dictionary, (2) a statistical inverse regression model to learn from the dictionary a probabilistic mapping between MR fingerprints and parameters, and (3) this mapping to provide both parameter estimates and their confidence levels. On synthetic data, experiments show that the quasi-random sampling outperforms the grid when designing the dictionary for inverse regression. Dictionaries up to 100 times smaller than usually employed in MRF yield more accurate parameter estimates with a 500 time gain. Estimates are supplied with a confidence index, well correlated with the estimation bias. On microvascular MRI data, results showed that dictionary-based methods (MRF and DBL) yield more accurate estimates than the conventional, closed-form equation, method. On MRI signals from tumor bearing rats, the DBL method shows very little sensitivity to the dictionary size in contrast to the MRF method. The proposed method efficiently reduces the number of required simulations to produce the dictionary, speeds up parameter estimation, and improve estimates accuracy. The DBL method also introduces a confidence index for each parameter estimate. Preliminary results have been presented at the third *Congrés National d'Imagerie du Vivant* (CNIV 2019) [53] and at the fourth *Congrés de la Société Française de Résonance Magnétique en Biologie et Médecine* (SFRMBM 2019) [54].

7.1.5. Characterization of daily glycemic variability in subjects with type 1 diabetes using a mixture of metrics

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 is an important component of glycemic control for patients with type 1 diabetes. 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. In a first study [24], our goal 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.

In a second study, we address the issue of choosing an appropriate measure of GV. Many metrics have been proposed to account for this variability but none is unanimous among physicians. The inadequacy of existing measurements lies in the fact that they view the variability from different aspects, so that no consensus has been reached among physicians as to which metrics to use in practice. Moreover, although glycemic variability, from one day to another, can show very different patterns, few metrics have been dedicated to daily evaluations. In this work [50], [30], a reference (stable-glycemia) statistical model is built based on a combination of daily computed canonical glycemic control metrics including variability. The metrics are computed for subjects from the TRIMECO islet transplantation trial , selected when their β-score (composite score for grading success) is greater than 6 after a transplantation. Then, for any new daily glycemia recording, its likelihood with respect to this reference model provides a multi-metric score of daily glycemic variability severity. In addition, determining the likelihood value that best separates the daily glycemia with a zero β-score from that greater than 6, we propose an objective decision rule to classify daily glycemia into "stable" or "unstable". The proposed characterization framework integrates multiple standard metrics and provides a comprehensive daily glycemic variability index, based on which, long term variability evaluations and investigations on the implicit link between variability and β-score can be carried out. Evaluation, in a daily glycemic variability classification task, shows that the proposed method is highly concordant to the experience of diabetologists. A multivariate statistical model is therefore proposed to characterize the daily glycemic variability of subjects with type 1 diabetes. The model has the advantage to provide a single variability score that gathers the information power of a number of canonical scores, too partial to be used individually. A reliable decision rule to classify daily variability measurements into stable or unstable is also provided.

7.1.6. Dirichlet process mixtures under affine transformations of the data

Participant: Julyan Arbel.

Joint work with: Riccardo Corradin and Bernardo Nipoti from Milano Bicocca, Italy.

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 [63], 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.

7.1.7. Approximate Bayesian computation via the energy statistic

Participants: Julyan Arbel, Florence Forbes, Hongliang Lu.

Joint work with: Hien Nguyen, La Trobe University Melbourne Australia.

Approximate Bayesian computation (ABC) has become an essential part of the Bayesian toolbox for addressing problems in which the likelihood is prohibitively expensive or entirely unknown, making it intractable. ABC defines a quasi-posterior by comparing observed data with simulated data, traditionally based on some summary statistics, the elicitation of which is regarded as a key difficulty. In recent years, a number of data discrepancy measures bypassing the construction of summary statistics have been proposed, including the Kullback-Leibler divergence, the Wasserstein distance and maximum mean discrepancies. In this work [79], we propose a novel importance-sampling (IS) ABC algorithm relying on the so-called two-sample energy statistic. We establish a new asymptotic result for the case where both the observed sample size and the simulated data sample size increase to infinity, which highlights to what extent the data discrepancy measure impacts the asymptotic pseudo-posterior. The result holds in the broad setting of IS-ABC methodologies, thus generalizing previous results that have been established only for rejection ABC algorithms. Furthermore, we propose a consistent V-statistic estimator of the energy statistic, under which we show that the large sample result holds. Our proposed energy statistic based ABC algorithm is demonstrated on a variety of models, including a Gaussian mixture, a moving-average model of order two, a bivariate beta and a multivariate g-and-k distribution. We find that our proposed method compares well with alternative discrepancy measures.

7.1.8. Industrial applications of mixture modeling

Participant: Julyan Arbel.

Joint work with: Kerrie Mengersen and Earl Duncan from QUT, School of Mathematical Sciences, Brisbane, Australia, and Clair Alston-Knox, Griffith University Brisbane, Australia, and Nicole White, Institute for Health and Biomedical Innovation, Brisbane, Australia.

In [61], 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. The first of these focuses on the iconic and pervasive need for process monitoring, and reviews a range of mixture approaches that have been proposed to tackle complex multimodal and dynamic or online processes. The second study reports on mixture approaches to resource allocation, applied here in a spatial health context but which are applicable more generally. The next study provides a more detailed description of a multivariate Gaussian mixture approach to a biosecurity risk assessment problem, using big data in the form of satellite imagery. This is followed by a final study that again provides a detailed description of a mixture model, this time using a nonparametric formulation, for assessing an industrial impact, notably the influence of a toxic spill on soil biodiversity.

7.2. Semi and non-parametric methods

7.2.1. Deep learning models to study the early stages of Parkinson's Disease

Participants: Florence Forbes, Veronica Munoz Ramirez, Virgilio Kmetzsch Rosa E Silva.

Joint work with: Michel Dojat from Grenoble Institute of Neuroscience.

Current physio-pathological data suggest that Parkinson's Disease (PD) symptoms are related to important alterations in subcortical brain structures. However, structural changes in these small structures remain difficult to detect for neuro-radiologists, in particular, at the early stages of the disease (*de novo* PD patients) [58], [43], [59]. The absence of a reliable ground truth at the voxel level prevents the application of traditional supervised deep learning techniques. In this work, we consider instead an anomaly detection approach and show that auto-encoders (AE) could provide an efficient anomaly scoring to discriminate *de novo* PD patients using quantitative Magnetic Resonance Imaging (MRI) data.

7.2.2. Estimation of extreme risk measures

Participants: Stephane Girard, Antoine Usseglio Carleve.

Joint work with: A. Daouia (Univ. Toulouse), L. Gardes (Univ. Strasbourg) 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.

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 [23], 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 [6]. 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. have recently received a lot of attention, especially in actuarial and financial risk man-agement. Their estimation, however, typically requires to consider non-explicit asymmetric leasts-quares estimates rather than the traditional order statistics used for quantile estimation. This makes the study of the tail expectile process a lot harder than that of the standard tail quantile process. Under the challenging model of heavy-tailed distributions, we derive joint weighted Gaussian approximations of the tail empirical expectile and quantile processes. We then use this powerful result to introduce and study new estimators of extreme expectiles and the standard quantile-based expected shortfall, as well as a novel expectile-based form of expected shortfall [22].

Both quantiles and expectiles were embedded in the more general class of L_p-quantiles [21] as the minimizers of a generic asymmetric convex loss function. It has been proved very recently that the only L_p-quantiles that are coherent risk measures are the expectiles. In [75], we work in a context of heavy tails, which is especially relevant to actuarial science, finance, econometrics and natural sciences, and we construct an estimator of the tail index of the underlying distribution based on extreme L_p-quantiles. We establish the asymptotic normality of such an estimator and in doing so, we extend very recent results on extreme expectile and L_p-quantile estimation. We provide a discussion of the choice of p in practice, as well as a methodology for reducing the bias of our estimator. Its finite-sample performance is evaluated on simulated data and on a set of real hydrological data. This work is submitted for publication.

7.2.3. Conditional extremal events

Participants: Stephane Girard, Antoine Usseglio Carleve.

Joint work with: G. Stupfler (Univ. Nottingham, UK), A. Ahmad, E. Deme and A. Diop (Université Gaston Berger, Sénégal).

The goal of the PhD thesis of Aboubacrene Ag Ahmad is to contribute to the development of theoretical and algorithmic models to tackle conditional extreme value analysis, *ie* the situation where some covariate information X is recorded simultaneously with a quantity of interest Y. In such a case, extreme quantiles and expectiles are functions of the covariate. In [13], we consider a location-scale model for conditional heavy-tailed distributions when the covariate is deterministic. First, nonparametric estimators of the location and scale functions are introduced. Second, an estimator of the conditional extreme-value index is derived. The asymptotic properties of the estimators are established under mild assumptions and their finite sample properties are illustrated both on simulated and real data.

As explained in Paragraph 7.2.2 , expectiles have recently started to be considered as serious candidates to become standard tools in actuarial and financial risk management. However, expectiles and their sample versions do not benefit from a simple explicit form, making their analysis significantly harder than that of quantiles and order statistics. This difficulty is compounded when one wishes to integrate auxiliary information about the phenomenon of interest through a finite-dimensional covariate, in which case the problem becomes the estimation of conditional expectiles. In [74], we exploit the fact that the expectiles of a distribution F are in fact the quantiles of another distribution E explicitly linked to F, in order to construct nonparametric kernel estimators of extreme conditional expectiles. We analyze the asymptotic properties of our estimators in the context of conditional heavy-tailed distributions. Applications to simulated data and real insurance data are provided. The results are submitted for publication.

7.2.4. Estimation of the variability in the distribution tail

Participant: Stephane Girard.

Joint work with: L. Gardes (Univ. Strasbourg).

We propose a new measure of variability in the tail of a distribution by applying a Box-Cox transformation of parameter $p \geq 0$ to the tail-Gini functional. It is shown that the so-called Box-Cox Tail Gini Variability measure is a valid variability measure whose condition of existence may be as weak as necessary thanks to the tuning parameter p. The tail behaviour of the measure is investigated under a general extreme-value condition on the distribution tail. We then show how to estimate the Box-Cox Tail Gini Variability measure within the range of the data. These methods provide us with basic estimators that are then extrapolated using the extreme-value assumption to estimate the variability in the very far tails. The finite sample behavior of the estimators is illustrated both on simulated and real data. This work is submitted for publication [72].

7.2.5. Extrapolation limits associated with extreme-value methods

Participant: Stephane 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 [15], 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 [14], 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.

7.2.6. Bayesian inference for copulas

Participants: Julyan Arbel, Marta Crispino, Stephane Girard.

We study in [16] 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.

7.2.7. Approximations of Bayesian nonparametric models

Participant: Julyan Arbel.

Joint work with: Stefano Favaro and Pierpaolo De Blasi from Collegio Carlo Alberto, Turin, Italy, Igor Prunster from Bocconi University, Milan, Italy, Caroline Lawless from Université Paris-Dauphine, France, Olivier Marchal from Université Jean Monnet.

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 [25] an elementary proof of Pitman–Yor's Chinese Restaurant process from its stick-breaking representation.

In [17], we consider approximations to the popular Pitman-Yor process obtained by truncating the stick-breaking representation. The truncation is determined by a random stopping rule that achieves an almost sure control on the approximation error in total variation distance. We derive the asymptotic distribution of the random truncation point as the approximation error goes to zero in terms of a polynomially tilted positive stable random variable. The practical usefulness and effectiveness of this theoretical result is demonstrated by devising a sampling algorithm to approximate functionals of the-version of the Pitman–Yor process.

In [18], we approximate predictive probabilities of Gibbs-type random probability measures, or Gibbs-type priors, which are arguably the most “natural” generalization of the celebrated Dirichlet prior. Among them the Pitman–Yor process certainly stands out for the mathematical tractability and interpretability of its predictive probabilities, which made it the natural candidate in several applications. Given a sample of size n, in this paper we show that the predictive probabilities of any Gibbs-type prior admit a large n approximation, with an error term vanishing as $o(1/n)$, which maintains the same desirable features as the predictive probabilities of the Pitman–Yor process.

In [18], we prove a monotonicity property of the Hurwitz zeta function which, in turn, translates into a chain of inequalities for polygamma functions of different orders. We provide a probabilistic interpretation of our result by exploiting a connection between Hurwitz zeta function and the cumulants of the exponential-beta distribution.

7.2.8. Concentration inequalities

Participant: Julyan Arbel.

Joint work with: Olivier Marchal from Université Jean Monnet and Hien Nguyen from La Trobe University Melbourne Australia.

In [19], we investigate the sub-Gaussian property for almost surely bounded random variables. If sub-Gaussianity per se is de facto ensured by the bounded support of said random variables, then exciting research avenues remain open. Among these questions is how to characterize the optimal sub-Gaussian proxy variance? Another question is how to characterize strict sub-Gaussianity, defined by a proxy variance equal to the (standard) variance? We address the questions in proposing conditions based on the study of functions variations. A particular focus is given to the relationship between strict sub-Gaussianity and symmetry of the distribution. In particular, we demonstrate that symmetry is neither sufficient nor necessary for strict sub-Gaussianity. In contrast, simple necessary conditions on the one hand, and simple sufficient conditions on the other hand, for strict sub-Gaussianity are provided. These results are illustrated via various applications to a number of bounded random variables, including Bernoulli, beta, binomial, uniform, Kumaraswamy, and triangular distributions.

7.2.9. Extraction and data analysis toward "industry of the future"

Participants: Florence Forbes, Hongliang Lu, Fatima Fofana.

Joint work with: J. F. Cuccaro and J. C Trochet from Vi-Technology company.

The overall idea of this project with Vi-Technology is to work towards manufacturing processes where machines communicate automatically so as to optimize the process performance as a whole. Starting from the assumption that transmitted information is essentially of statistical nature, the role of MISTIS in this context was to identify what statistical methods might be useful for the printed circuits boards assembly industry. A first step was to extract and analyze data from two inspection machines in an industrial process making electronic cards. After a first extraction 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 had access to two databases at both ends (SPI and Component Inspection) of the assembly process. The goal was 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.

7.2.10. Tracking and analysis of large population of dynamic single molecules

Participant: Florence Forbes.

Joint work with: Virginie Stoppin-Mellet from Grenoble Institute of Neuroscience, Vincent Brault from Laboratoire Jean Kuntzmann, Emilie Lebarbier from Nanterre University and Guy Bendao from AgroParisTech.

In the last decade, the number of studies using single molecule approaches has increased significantly. Thanks to technological progress and in particular with the development of TIRFM (Total Internal Reflection Fluorescence Microscopy), biologists can now observe single molecules at work. However, real time single molecule approaches remain mastered by a limited number of labs, and challenging obstacles have to be overcome before it becomes more broadly accessible. One important issue is the efficient detection and tracking of individual molecules in noisy images (low signal-to-noise ratio, SNR). Considering for example a TIRFM movie where single molecules stochastically appear and disappear at random positions, the low SNR implies that each individual molecule has to be detected at sub-pixel resolution over its local background and that this operation has to be repeated on each frame of the movie, thus requiring considerable amount of calculations. Procedures to detect single molecules are available, but they are mostly applicable to immobile molecules, are not statistically robust, and they often require an image processing that alters the quantitative signal information. In particular the intensity of a signal might be modified so that it becomes difficult to know the number of molecules associated with a specific signal. Crucial information such as the stoichiometry of the molecular complexes are then lost. Another challenging issue concerns data processing. Molecule tracking generate traces of time-dependent intensity fluctuations for each molecule. But single traces contain limited amount of information, and thus a very large number of traces must be analysed to extract general rules. In this context, the first aim of the present project was to provide a general procedure to track in real time transient interactions of a large number of biological molecules observed with TIRF microscopy and to generate traces of time-dependent intensity fluctuations. The second aim was to define a robust statistical approach to detect discrete events in a noisy time-dependent signal and extract parameters that describe the kinetics of these events. For this task we gathered expertise from biology (Grenoble Institute of Neuroscience) and statistics (Inria Mistis, LJK and AgroParisTech) in the context of a multidisciplinary project funded by the Grenoble data institute for 2 years.

7.3. Graphical and Markov models

7.3.1. Structure learning via Hadamard product of correlation and partial correlation matrices

Participants: Sophie Achard, Karina Ashurbekova, Florence Forbes.

Structure learning is an active topic nowadays in different application areas, i.e. genetics, neuroscience. Classical conditional independences or marginal independences may not be sufficient to express complex relationships. This work [39] is introducing a new structure learning procedure where an edge in the graph corresponds to a non zero value of both correlation and partial correlation. Based on this new paradigm, we define an estimator and derive its theoretical properties. The asymptotic convergence of the proposed graph estimator and its rate are derived. Illustrations on a synthetic example and application to brain connectivity are displayed.

7.3.2. Optimal shrinkage for robust covariance matrix estimators in a small sample size setting

Participants: Sophie Achard, Karina Ashurbekova, Florence Forbes, Antoine Usseglio Carleve.

When estimating covariance matrices, traditional sample covariance-based estimators are straightforward but suffer from two main issues: 1) a lack of robustness, which occurs as soon as the samples do not come from a Gaussian distribution or are contaminated with outliers and 2) a lack of data when the number of parameters to estimate is too large compared to the number of available observations, which occurs as soon as the covariance matrix dimension is greater than the sample size. The first issue can be handled by assuming samples are drawn from a heavy-tailed distribution, at the cost of more complex derivations, while the second issue can be addressed by shrinkage with the difficulty of choosing the appropriate level of regularization. In this work [66] we offer both a tractable and optimal framework based on shrinked likelihood-based M-estimators. First, a closed-form expression is provided for a regularized covariance matrix estimator with an optimal shrinkage coefficient for any sample distribution in the elliptical family. Then, a complete inference procedure is proposed which can also handle both unknown mean and tail parameter, in contrast to most existing methods that focus on the covariance matrix parameter requiring pre-set values for the others. An illustration on synthetic and real data is provided in the case of the t-distribution with unknown mean and degrees-of-freedom parameters.

7.3.3. Robust penalized inference for Gaussian Scale Mixtures

Participants: Sophie Achard, Karina Ashurbekova, Florence Forbes.

The literature on sparse precision matrix estimation is rapidly growing. Many strong methods are valid only for Gaussian variables. One of the most commonly used approaches in this case is glasso which aims to minimize the negative L1-penalized log-likelihood function. In practice, data may deviate from normality in various ways, outliers and heavy tails frequently occur that can severely degrade the Gaussian models performance. A natural solution is to turn to heavier tailed distributions that remain tractable. For this purpose, we propose [51] a penalized version of the EM algorithm for Gaussian Scale Mixtures.

7.3.4. Non parametric Bayesian priors for graph structured data

Participants: Florence Forbes, Julyan Arbel, Hongliang Lu.

We consider the issue of determining the structure of clustered data, both in terms of finding the appropriate number of clusters and of modelling the right dependence structure between the observations. Bayesian nonparametric (BNP) models, which do not impose an upper limit on the number of clusters, are appropriate to avoid the required guess on the number of clusters but have been mainly developed for independent data. In contrast, Markov random fields (MRF) have been extensively used to model dependencies in a tractable manner but usually reduce to finite cluster numbers when clustering tasks are addressed. Our main contribution is to propose a general scheme to design tractable BNP-MRF priors that combine both features: no commitment to an arbitrary number of clusters and a dependence modelling. A key ingredient in this construction is the availability of a stick-breaking representation which has the threefold advantage to allowing us to extend standard discrete MRFs to infinite state space, to design a tractable estimation algorithm using variational approximation and to derive theoretical properties on the predictive distribution and the number of clusters of the proposed model. This approach is illustrated on a challenging natural image segmentation task for which it shows good performance with respect to the literature. This work [77] will be presented as a poster at BayesComp2020 in Gainesville, Florida, USA, [78].

7.3.5. Bayesian nonparametric models for hidden Markov random fields on count variables and application to disease mapping

Participants: Julyan Arbel, Fatoumata Dama, Jean-Baptiste Durand, Florence Forbes.

Hidden Markov random fields (HMRFs) have been widely used in image segmentation and more generally, for clustering of data indexed by graphs. Dependent hidden variables (states) represent the cluster identities and determine their interpretations. Dependencies between state variables are induced by the notion of neighborhood in the graph. A difficult and crucial problem in HMRFs is the identification of the number of possible states K. Recently, selection methods based on Bayesian non parametric priors (Dirichlet processes) have been developed. They do not assume that K is bounded a priori, thus allowing its adaptive selection with respect to the quantity of available data and avoiding costly systematic estimation and comparison of models with different fixed values for K. Our previous work [77] has focused on Bayesian nonparametric priors for HMRFs and continuous, Gaussian observations. In this work, we consider extensions to discrete observed data typically issued from counts. We define and implement Bayesian nonparametric models for HMRFs with Poisson distributed observations. As an illustration, we propose a new disease mapping model for epidemiology. The inference is done by Variational Bayesian Expectation Maximization (VBEM). Results on synthetic data sets suggest that our model is able to recover the true number of risk levels (clusters) and to provide a good estimation of the true risk level partition. Application on real data then also shows satisfying results.

As a perspective, Bayesian nonparametric models for hidden Markov random fields could be extended to non-Poissonian models (particularly to account for zero-inflated and over-/under-dispersed cases of application) and to regression models.

7.3.6. Hidden Markov models for the analysis of eye movements

Participants: Jean-Baptiste Durand, Brice Olivier, Sophie Achard.

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 strategies or 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) [86], but we used hidden semi-Markov models for better characterization of phase length distributions (Olivier *et al.*, 2017) [85]. The estimated HMM highlighted contrasted reading strategies, with both individual and document-related variability. 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.

Then, using the restored state values, statistical characteristics of EEGs were compared according to strategies, brain wave frequencies and EEG channels (i.e., location on scalp). Differences in variance and correlations related to strategy changes were highlighted. Dependency graphs interpreted as maps of functional brain connectivity were estimated for each strategy and frequency and their changes were interpreted.

These results were published in Brice Olivier's PhD manuscript [12]. Although the approach was sufficient to highlight significant discrimination of strategies, it suffered from somewhat overlapping eye-movement characteristics over strategies. As a result, high uncertainty in the phase changes arose, which could induce underestimation of EEG and eye movement abilities to discriminate strategies.

This is why we developed integrated models coupling EEG and eye movements within one single HMM for better identification of strategies. Here, the coupling incorporated some delay between transitions in both EEG and eye-movement state sequences, since EEG patterns associated to cognitive processes occur lately with respect to eye-movement state switches. 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.

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 reading strategies.

7.3.7. Comparison of initialization strategies in the EM algorithm for hidden Semi-Markov processes

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)

In Subsection 7.3.6 , hidden semi-Markov models (HSMMs) were used to infer reading strategies from eye-movement and EEG time series. Model parameters were estimated by the EM algorithm. Its principle is to build a sequence of parameters with increasing likelihood values, starting from a starting point. The impact of this starting point has not been investigated in the case of HSMMs; this is why we aimed at developing and assessing an initialization method based on the available sequence lengths [48]. This consists in randomly choosing a number of transitions and then, uniformly-distributed transition times given the number of transitions. These transition times break the sequences into segements and assign uniformly-distributed states to each segment with the constraint that two consecutive states should be different.

The method was compared to other initialization strategies and was shown to be efficient on several data sets with multiple categorical sequences.

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 [40], 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. Bayesian neural networks

Participants: Julyan Arbel, Mariia Vladimirova.

Joint work with: Pablo Mesejo from University of Granada, Spain, Jakob Verbeek from Inria Grenoble Rhône-Alpes, France.

We investigate in [45] 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/she 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 was published in an international journal in 2018 and leads to a keynote as an invited speaker to the 12th Scientific Meeting Classification and Data Analysis Group Cassino (CLADAG 2019) in Italy [41].

It is a joint work with Alexandre Lourme from University of Bordeaux.

7.2. 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 accepted in an international journal [28]. The related R package ordinalClust has been also written and has led to a specific preprint [73] now submitted to an international journal.

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.

7.3. 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 now accepted in an international journal [29].

This is joint work with Margot Selosse (PhD student) and Julien Jacques, both from University of Lyon 2.

7.4. 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 illustration and comparison with traditional co-clustering. This work has been submitted to an international journal [63].

This is a joint work with Michael Gallaugher (PhD student) and Paul McNicholas, both from McMaster University (Canada). Michael Gallaugher visited Modal for three months in 2018.

7.5. 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 is now in minor revision for an international journal [54]. It has also led to an invited talk to an international conference [42], and several other invitations (the workshop “Advances in data science for big and complex data” at Université Paris-Dauphine in January and the seminary of the Probability and Statistics team of the University Nice Sophia-Antipolis in November).

This is a joint work with Matthieu Marbac from ENSAI.

7.6. Axis 1: Co-clustering: A versatile way to perform clustering

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 the latent bloc model, a probabilistic model for co-clustering, is of particular interest to perform HD clustering of individuals even if it is not its primary function. We illustrate in an empirical manner the trade-off bias-variance of the co-clustering strategy in scenarii involving HD fundaments (correlated variables, irrelevant variables) and show the ability of co-clustering to outperform simple mixture row-clustering. An early version of this work has been presented to an national conference with international audience [46].

We also co-organized a special session to an international conference [45] to discuss the potential links between deterministic methods for co-clustering (based on a metric and computer science procedure) or probabilistic methods for co-clustering (mainly based on mixture models). It was the opportunity to gather related communities which are often distinct.

All are joint works with Christine Keribin from Université Paris-Sud.

7.7. 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. This work has been presented as an invited speaker to an international conference [31]. It has also been presented at a national conference with international audience [47] and as a poster to the international Working Group on Model-Based Clustering [69]. Currently, a preprint is being finalized for submission to an international journal.

It is a joint work with Gilles Celeux from Inria Saclay and Julie Josse from Ecole Polytechnique.

7.8. Axis 1: Organized Co-Clustering 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 paper is currently in revision in an international journal [72].

This is joint work with Margot Selosse (PhD student) and Julien Jacques, both from University of Lyon 2.

7.9. 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. An article has been submitted to *Journal of Classification* and should incorporate “Major Revisions”.

7.10. 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 still an ongoing work, with several short working papers.

It is a joint work with Alexandre Lourme from University of Bordeaux.

7.11. Axis 1: Predictive clustering

Participants: Christophe Biernacki, Vincent Vandewalle.

Many data, for instance in biostatistics, contain some sets of variables which permit evaluating unobserved traits of the subjects (e.g., we ask question about how many pizzas, hamburgers, chips... are eaten to know how healthy are the food habits of the subjects). Moreover, we often want to measure the relations between these unobserved traits and some target variables (e.g., obesity). Thus, a two-steps procedure is often used: first, a clustering of the observations is performed on the sets of variables related to the same topic; second, the predictive model is fitted by plugging the estimated partitions as covariates. Generally, the estimated partitions are not exactly equal to the true ones. We investigate the impact of these measurement errors on the estimators of the regression parameters, and we explain when this two-steps procedure is consistent. We also present a specific EM algorithm which simultaneously estimates the parameters of the clustering and predictive models. It is an ongoing work.

It is a joint work with Matthieu Marbac from ENSAI and Mohammed Sedki from University Paris-Sud.

7.12. Axis 1: Ranking and synchronization from pairwise measurements via SVD

Participant: Hemant Tyagi.

Given a measurement graph $G = ([n], E)$ and an unknown signal $r \in R^n$, we investigate algorithms for recovering r from pairwise measurements of the form $r_i - r_j$; $\{i, j\} \in E$. This problem arises in a variety of applications, such as ranking teams in sports data and time synchronization of distributed networks. Framed in the context of ranking, the task is to recover the ranking of n teams (induced by r) given a small subset of noisy pairwise rank offsets. We propose a simple SVD-based algorithmic pipeline for both the problem of time synchronization and ranking. We provide a detailed theoretical analysis in terms of robustness against both sampling sparsity and noise perturbations with outliers, using results from matrix perturbation and random matrix theory. Our theoretical findings are complemented by a detailed set of numerical experiments on both synthetic and real data, showcasing the competitiveness of our proposed algorithms with other state-of-the-art methods.

This is joint work with Alexandre d'Aspremont (CNRS & ENS, Paris) and Mihai Cucuringu (University of Oxford, UK) and is available as a preprint [61].

7.13. Axis 1: SPONGE: A generalized eigenproblem for clustering signed networks

Participant: Hemant Tyagi.

We introduce a principled and theoretically sound spectral method for k-way clustering in signed graphs, where the affinity measure between nodes takes either positive or negative values. Our approach is motivated by social balance theory, where the task of clustering aims to decompose the network into disjoint groups, such that individuals within the same group are connected by as many positive edges as possible, while individuals from different groups are connected by as many negative edges as possible. Our algorithm relies on a generalized eigenproblem formulation inspired by recent work on constrained clustering. We provide theoretical guarantees for our approach in the setting of a signed stochastic block model, by leveraging tools from matrix perturbation theory and random matrix theory. An extensive set of numerical experiments on both synthetic and real data shows that our approach compares favorably with state-of-the-art methods for signed clustering, especially for large number of clusters and sparse measurement graphs.

This is joint work with Mihai Cucuringu (University of Oxford, UK), Peter Davies (University of Warwick, UK) and Aldo Glielmo (Imperial College, London, UK) and was mostly done while Hemant Tyagi was affiliated to the Alan Turing Institute. It was published in the proceedings of an international conference [32].

7.14. Axis 2: Multi-kernel unmixing and super-resolution using the Modified Matrix Pencil method

Participant: Hemant Tyagi.

Consider L groups of point sources or spike trains, with the l^{th} group represented by $x_l(t)$. For a function $g: R \to R$, let $g_l(t) = g(t/\mu_l)$ denote a point spread function with scale $\mu_l > 0$, and with $\mu_1 < \cdots < \mu_L$. With $y(t) = \sum_{l=1}^{L} (g_l \star x_l)(t)$, our goal is to recover the source parameters given samples of y, or given the Fourier samples of y. This problem is a generalization of the usual super-resolution setup wherein $L = 1$; we call this the multi-kernel unmixing super-resolution problem. Assuming access to Fourier samples of y, we derive an algorithm for this problem for estimating the source parameters of each group, along with precise non-asymptotic guarantees. Our approach involves estimating the group parameters sequentially in the order of increasing scale parameters, i.e., from group 1 to L. In particular, the estimation process at stage $1 \leq l \leq L$ involves (i) carefully sampling the tail of the Fourier transform of y, (ii) a *deflation* step wherein we subtract the contribution of the groups processed thus far from the obtained Fourier samples, and (iii) applying Moitra's modified Matrix Pencil method on a deconvolved version of the samples in (ii).

This is joint work with Stephane Chretien (National Physical Laboratory, UK & Alan Turing Institute, London) and was mostly done while Hemant Tyagi was affiliated to the Alan Turing Institute. It is currently under revision in an international journal and is available as a preprint [56].

7.15. Axis 2: Provably robust estimation of modulo 1 samples of a smooth function with applications to phase unwrapping

Participant: Hemant Tyagi.

Consider an unknown smooth function $f : [0,1]^d \to R$, and assume we are given n noisy mod 1 samples of f, i.e., $y_i = (f(x_i) + \eta_i) \mod 1$, for $x_i \in [0,1]^d$, where η_i denotes the noise. Given the samples $(x_i, y_i)_{i=1}^n$, our goal is to recover smooth, robust estimates of the clean samples $f(x_i) \mod 1$. We formulate a natural approach for solving this problem, which works with angular embeddings of the noisy mod 1 samples over the unit circle, inspired by the angular synchronization framework. This amounts to solving a smoothness regularized least-squares problem – a quadratically constrained quadratic program (QCQP) – where the variables are constrained to lie on the unit circle. Our proposed approach is based on solving its relaxation, which is a *trust-region sub-problem* and hence solvable efficiently. We provide theoretical guarantees demonstrating its robustness to noise for adversarial, as well as random Gaussian and Bernoulli noise models. To the best of our knowledge, these are the first such theoretical results for this problem. We demonstrate the robustness and efficiency of our proposed approach via extensive numerical simulations on synthetic data, along with a simple least-squares based solution for the unwrapping stage, that recovers the original samples of f (up to a global shift). It is shown to perform well at high levels of noise, when taking as input the denoised modulo 1 samples. Finally, we also consider two other approaches for denoising the modulo 1 samples that leverage tools from Riemannian optimization on manifolds, including a Burer-Monteiro approach for a semidefinite programming relaxation of our formulation. For the two-dimensional version of the problem, which has applications in synthetic aperture radar interferometry (InSAR), we are able to solve instances of real-world data with a million sample points in under 10 seconds, on a personal laptop.

This is joint work with Mihai Cucuringu (University of Oxford, UK) and was mostly done while Hemant Tyagi was affiliated to the Alan Turing Institute. It has been accepted to appear (after minor revision) in an international journal, and is available as a preprint [60].

7.16. Axis 2: Learning general sparse additive models from point queries in high dimensions

Participant: Hemant Tyagi.

We consider the problem of learning a d-variate function f defined on the cube $[-1,1]^d \subset R^d$, where the algorithm is assumed to have black box access to samples of f within this domain. Denote $S_r; r = 1, \cdots, r_0$ to be sets consisting of unknown r-wise interactions amongst the coordinate variables. We then focus on the setting where f has an additive structure, i.e., it can be represented as

$$f = \sum_{j \in \S_1} \phi_j + \sum_{j \in S_2} \phi_j + \cdots + \sum_{j \in S_{r_0}} \phi_j,$$

where each ϕ_j; $j \in S_r$ is at most r-variate for $1 \leq r \leq r_0$. We derive randomized algorithms that query f at carefully constructed set of points, and exactly recover each S_r with high probability. In contrary to the previous work, our analysis does not rely on numerical approximation of derivatives by finite order differences.

This is joint work with Jan Vybiral (Czech Technical University, Prague) and was mostly done while Hemant Tyagi was affiliated to the Alan Turing Institute. It has now been published in an international journal [30].

7.17. Axis 2: Sparse non-negative super-resolution - simplified and stabilized

Participant: Hemant Tyagi.

The convolution of a discrete measure, $x = \sum_{i=1}^{k} a_i \delta_{t_i}$, with a local window function, $\phi(s-t)$, is a common model for a measurement device whose resolution is substantially lower than that of the objects being observed. Super-resolution concerns localising the point sources with an accuracy beyond the essential support of $\phi(s-t)$, typically from m noisy samples of the convolution output. We consider the setting of x being non-negative and seek to characterise all non-negative measures approximately consistent with the samples. We first show that x is the unique non-negative measure consistent with the samples provided the samples are exact, and $m \geq 2k+1$ samples are available, and $\phi(s-t)$ generates a Chebyshev system. This is independent of how close the sample locations are and *does not rely on any regulariser beyond non-negativity*; as such, it extends and clarifies the work by Schiebinger et al. and De Castro et al., who achieve the same results but require a total variation regulariser, which we show is unnecessary. Moreover, we establish stability results in the setting where the samples are corrupted with noise. The main innovation of these results is that non-negativity alone is sufficient to localise point sources beyond the essential sensor resolution.

This is joint work with Armin Eftekhari (EPFL, Switzerland), Jared Tanner (University of Oxford, UK), Andrew Thompson (National Physical Laboratory, UK), Bogdan Toader (University of Oxford, UK) and was mostly done while Hemant Tyagi was affiliated to the Alan Turing Institute. It has now been published in an international journal [24].

7.18. Axis 2: Pseudo-Bayesian learning with kernel Fourier transform as prior

Participant: Pascal Germain.

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 joint work with Emilie Morvant from Université Jean Monnet de Saint-Etienne (France), and Gaël Letarte from Université Laval (Québec, Canada) has been initiated in 2018 when Gaël Letarte was doing an internship at Inria, and led to a publication in the proceedings of AISTATS 2019 conference [36]. The same work has been prensented as a poster in the "Workshop on Machine Learning with guarantees @ NeurIPS 2019".

An extension of this work, co-authored with Léo Gautheron, Amaury Habrard, Marc Sebban, and Valentina Zantedeschi – all from Université Jean Monnet de Saint-Etienne – has been presented at the national conference CAp 2019 [44]. It is also the topic of a technical report [64].

7.19. Axis 2: PAC-Bayesian binary activated deep neural networks

Participant: Pascal Germain, Benjamin Guedj

We present a comprehensive study of multilayer neural networks with binary activation, relying on the PAC-Bayesian theory. Our contributions are twofold: (i) we develop an end-to-end framework to train a binary activated deep neural network, overcoming the fact that binary activation function is non-differentiable; (ii) we provide nonvacuous PAC-Bayesian generalization bounds for binary activated deep neural networks. Noteworthy, our results are obtained by minimizing the expected loss of an architecture-dependent aggregation of binary activated deep neural networks. The performance of our approach is assessed on a thorough numerical experiment protocol on real-life datasets. This work has been published in the proceedings of NeurIPS 2019 conference [35].

It is a joint work with Gaël Letarte and François Laviolette, from Université Laval (Québec, Canada).

7.20. Axis 2: Improved PAC-Bayesian Bounds for Linear Regression

Participant: Pascal Germain, Vera Shalaeva

We improve the PAC-Bayesian error bound for linear regression provided in the literature. The improvements are two-fold. First, the proposed error bound is tighter, and converges to the generalization loss with a well-chosen temperature parameter. Second, the error bound also holds for training data that are not independently sampled. In particular, the error bound applies to certain time series generated by well-known classes of dynamical models, such as ARX models.

It is a joint work with Mihaly Petreczky and Alireza Fakhrizadeh Esfahani from Université de Lille. It has been accepted for publication as part of the AAAI 2020 conference [38].

7.21. Axis 2: Multiview Boosting by controlling the diversity and the accuracy of view-specific voters

Participant: Pascal Germain

We present a comprehensive study of multilayer neural networks with binary activation, relying on the PAC-Bayesian 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.

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. This work has been published in the journal Neurocomputing [26].

7.22. Axis 2: PAC-Bayes and Domain Adaptation

Participant: Pascal Germain

In machine learning, Domain Adaptation (DA) arises when the distribution generating the test (target) data differs from the one generating the learning (source) data. It is well known that DA is a hard task even under strong assumptions, among which the covariate-shift where the source and target distributions diverge only in their marginals, i.e. they have the same labeling function. Another popular approach is to consider a hypothesis class that moves closer the two distributions while implying a low-error for both tasks. This is a VC-dim approach that restricts the complexity of a hypothesis class in order to get good generalization. Instead, we propose a PAC-Bayesian approach that seeks for suitable weights to be given to each hypothesis in order to build a majority vote. We prove a new DA bound in the PAC-Bayesian context. This leads us to design the first DA-PAC-Bayesian algorithm based on the minimization of the proposed bound. Doing so, we seek for a ρ-weighted majority vote that takes into account a trade-off between three quantities. The first two quantities being, as usual in the PAC-Bayesian approach, (a) the complexity of the majority vote (measured by a Kullback-Leibler divergence) and (b) its empirical risk (measured by the ρ-average errors on the source sample). The third quantity is (c) the capacity of the majority vote to distinguish some structural difference between the source and target samples.

This work has been published in the journal Neurocomputing [25].

It is a joint work with Emilie Morvant and Amaury Habrard from Université Jean Monnet de Saint-Etienne (France), and with François Laviolette from Université Laval (Québec, Canada).

7.23. Axis 2: Interpreting Neural Networks as Majority Votes through the PAC-Bayesian Theory

Participant: Pascal Germain, Paul Viallard

We propose a PAC-Bayesian theoretical study of the two-phase learning procedure of a neural network introduced by Kawaguchi et al. (2017). In this procedure, a network is expressed as a weighted combination of all the paths of the network (from the input layer to the output one), that we reformulate as a PAC-Bayesian majority vote. Starting from this observation, their learning procedure consists in (1) learning “prior” network for fixing some parameters, then (2) learning a “posterior” network by only allowing a modification of the weights over the paths of the prior network. This allows us to derive a PAC-Bayesian generalization bound that involves the empirical individual risks of the paths (known as the Gibbs risk) and the empirical diversity between pairs of paths. Note that similarly to classical PAC-Bayesian bounds, our result involves a KL-divergence term between a “prior” network and the "posterior" network. We show that this term is computable by dynamic programming without assuming any distribution on the network weights.

This early result has been accepted as a poster presentation in the international workshop “Workshop on Machine Learning with guarantees @ NeurIPS 2019” [50].

This is a joint work with researchers from Université Jean Monnet de Saint-Etienne: Amaury Habrard, Emilie Morvant, and Rémi Emonet.

7.24. Axis 2: Still no free lunches: the price to pay for tighter PAC-Bayes bounds

Participant: Benjamin Guedj

“No free lunch” results state the impossibility of obtaining meaningful bounds on the error of a learning algorithm without prior assumptions and modelling. Some models are expensive (strong assumptions, such as as subgaussian tails), others are cheap (simply finite variance). As it is well known, the more you pay, the more you get: in other words, the most expensive models yield the more interesting bounds. Recent advances in robust statistics have investigated procedures to obtain tight bounds while keeping the cost minimal. The present paper explores and exhibits what the limits are for obtaining tight PAC-Bayes bounds in a robust setting for cheap models, addressing the question: is PAC-Bayes good value for money?

Joint work with Louis Pujol (Université Paris-Saclay). Available as a preprint: [68]

7.25. Axis 2: PAC-Bayesian Contrastive Unsupervised Representation Learning

Participant: Benjamin Guedj, Pascal Germain

Contrastive unsupervised representation learning (CURL) is the state-of-the-art technique to learn representations (as a set of features) from unlabelled data. While CURL has collected several empirical successes recently, theoretical understanding of its performance was still missing. In a recent work, Arora et al. (2019) provide the first generalisation bounds for CURL, relying on a Rademacher complexity. We extend their framework to the flexible PAC-Bayes setting, allowing to deal with the non-iid setting. We present PAC-Bayesian generalisation bounds for CURL, which are then used to derive a new representation learning algorithm. Numerical experiments on real-life datasets illustrate that our algorithm achieves competitive accuracy, and yields generalisation bounds with non-vacuous values.

Joint work with Kento Nozawa (University of Tokyo & RIKEN). Available as a preprint: [71]

7.26. Axis 2: Sequential Learning of Principal Curves: Summarizing Data Streams on the Fly

Participant: Benjamin Guedj

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 (called `slpc`, for Sequential Learning Principal Curves) that incorporates both sleeping experts and multi-armed bandit ingredients is presented, along with its regret computation and performance on synthetic and real-life data.

Joint work with Le Li (Université d'Angers & iAdvize). Available as a preprint: [67]

7.27. Axis 2: PAC-Bayes Un-Expected Bernstein Inequality

Participant: Benjamin Guedj

We present a new PAC-Bayesian generalization bound. Standard bounds contain a $\sqrt{L_n \cdot KL/n}$ complexity term which dominates unless L_n, the empirical error of the learning algorithm's randomized predictions, vanishes. We manage to replace L_n by a term which vanishes in many more situations, essentially whenever the employed learning algorithm is sufficiently stable on the dataset at hand. Our new bound consistently beats state-of-the-art bounds both on a toy example and on UCI datasets (with large enough n). Theoretically, unlike existing bounds, our new bound can be expected to converge to 0 faster whenever a Bernstein/Tsybakov condition holds, thus connecting PAC-Bayesian generalization and *excess risk* bounds—for the latter it has long been known that faster convergence can be obtained under Bernstein conditions. Our main technical tool is a new concentration inequality which is like Bernstein's but with X^2 taken outside its expectation.

Joint work with Peter Grünwald (CWI), Zakaria Mhammedi (Australian National University).

This work has been accepted at NeurIPS 2019, will be presented as a poster in the main conference and as a oral in the workshop "Machine Learning with guarantees", and is included in the proceedings of NeurIPS 2019.

Published: [37]

7.28. Axis 2: Attributing and Referencing (Research) Software: Best Practices and Outlook from Inria

Participant: Benjamin Guedj

Software is a fundamental pillar of modern scientiic research, not only in computer science, but actually across all elds and disciplines. However, there is a lack of adequate means to cite and reference software, for many reasons. An obvious rst reason is software authorship, which can range from a single developer to a whole team, and can even vary in time. The panorama is even more complex than that, because many roles can be involved in software development: software architect, coder, debugger, tester, team manager, and so on. Arguably, the researchers who have invented the key algorithms underlying the software can also claim a part of the authorship. And there are many other reasons that make this issue complex. We provide in this paper a contribution to the ongoing eeorts to develop proper guidelines and recommendations for software citation, building upon the internal experience of Inria, the French research institute for digital sciences. As a central contribution, we make three key recommendations. (1) We propose a richer taxonomy for software contributions with a qualitative scale. (2) We claim that it is essential to put the human at the heart of the evaluation. And (3) we propose to distinguish citation from reference.

Joint work with Pierre Alliez, Roberto Di Cosmo, Alain Girault, Mohand-Said Hacid, Arnaud Legrand, Nicolas Rougier (Inria).

This work has been published in the journal Computing in Science and Engineering.

Published: [14]

7.29. Axis 2: Revisiting clustering as matrix factorisation on the Stiefel manifold

Participant: Benjamin Guedj

This paper studies clustering for possibly high dimensional data (*e.g.* images, time series, gene expression data, and many other settings), and rephrase it as low rank matrix estimation in the PAC-Bayesian framework. Our approach leverages the well known Burer-Monteiro factorisation strategy from large scale optimisation, in the context of low rank estimation. Moreover, our Burer-Monteiro factors are shown to lie on a Stiefel manifold. We propose a new generalized Bayesian estimator for this problem and prove novel prediction bounds for clustering. We also devise a componentwise Langevin sampler on the Stiefel manifold to compute this estimator.

Joint work with Stéphane Chrétien (Université Lyon-2). Available as a preprint: [55]

7.30. Axis 2: A Primer on PAC-Bayesian Learning

Participant: Benjamin Guedj

This survey on PAC-Bayesian learning has been the backbone to a successful proposal for an ICML 2019 plenary tutorial.

Generalised Bayesian learning algorithms are increasingly popular in machine learning, due to their PAC generalisation properties and flexibility. The present paper aims at providing a self-contained survey on the resulting PAC-Bayes framework and some of its main theoretical and algorithmic developments.

This work has been published in the proceedings of the French Mathematical Society. Published as [66].

7.31. Axis 2: Perturbed Model Validation: A New Framework to Validate Model Relevance

Participant: Benjamin Guedj

This paper introduces Perturbed Model Validation (PMV), a new technique to validate model relevance and detect overfitting or underfitting. PMV operates by injecting noise to the training data, re-training the model against the perturbed data, then using the training accuracy decrease rate to assess model relevance. A larger decrease rate indicates better concept-hypothesis fit. We realise PMV by perturbing labels to inject noise, and evaluate PMV on four real-world datasets (breast cancer, adult, connect-4, and MNIST) and nine synthetic datasets in the classification setting. The results reveal that PMV selects models more precisely and in a more stable way than cross-validation, and effectively detects both overfitting and underfitting.

It is a joint work with Jie Zhang, Earl Barr, John Shawe-Taylor (all with UCL), and Mark Harman (UCL & Facebook). Available as a preprint: [75].

7.32. 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 cannot share data but instead share their models. Models are shared only one time so as to preserve the network load. We introduce DELCO (standing for Decentralized Ensemble Learning with COpulas), a new approach allowing to aggregate the predictions of the classifiers trained by each learner. 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 in case of dependent classifiers. A companion python implementation is available online.

Joint work with John Klein, Olivier Colot, Mahmoud Albardan (Université de Lille).

This work has been published in the proceedings of ECML-PKDD 2019, as part (oral presentation) of the workshop Decentralized Machine Learning at the Edge. Published: [34]

7.33. Axis 2: Online k-means Clustering

Participant: Benjamin Guedj

We study the problem of online clustering where a clustering algorithm has to assign a new point that arrives to one of k clusters. The specific formulation we use is the k-means objective: At each time step the algorithm has to maintain a set of k candidate centers and the loss incurred is the squared distance between the new point and the closest center. The goal is to minimize regret with respect to the best solution to the k-means objective ($\mathcal{C}$) in hindsight. We show that provided the data lies in a bounded region, an implementation of the Multiplicative Weights Update Algorithm (*MWUA*) using a discretized grid achieves a regret bound of $\widetilde{O}(\sqrt{T})$ in expectation. We also present an online-to-offline reduction that shows that an efficient no-regret online algorithm (despite being allowed to choose a different set of candidate centres at each round) implies an offline efficient algorithm for the k-means problem. In light of this hardness, we consider the slightly weaker requirement of comparing regret with respect to $(1+\epsilon)\mathcal{C}$ and present a no-regret algorithm with runtime $O\left(T(\mathrm{poly}(\log(T), k, d, 1/\epsilon)^{k(d+O(1))}\right)$. Our algorithm is based on maintaining an incremental coreset and an adaptive variant of the *MWUA*. We show that naïve online algorithms, such as *Follow The Leader*, fail to produce sublinear regret in the worst case. We also report preliminary experiments with synthetic and real-world data.

Joint work with Varun Kanade, Guy Rom (University of Oxford), Vincent Cohen-Addad (CNRS). Available as a preprint: [57]

7.34. Axis 2: Non-linear aggregation of filters to improve image denoising

Participant: Benjamin Guedj

We introduce a novel aggregation method to efficiently perform image denoising. Preliminary filters are aggregated in a non-linear fashion, using a new metric of pixel proximity based on how the pool of filters reaches a consensus. We provide a theoretical bound to support our aggregation scheme, its numerical performance is illustrated and we show that the aggregate significantly outperforms each of the preliminary filters.

Joint work with Juliette Rengot (Ecole des Ponts).

This work has been accepted at the Computing Conference 2020 (July 2020, London, UK) and will be included in the proceedings. Published: [33]

7.35. Axis 2: Multiple change-points detection with reproducing kernels

Participant: Alain Celisse

We tackle the change-point problem with data belonging to a general set. We build a penalty for choosing the number of change-points in the kernel-based method of Harchaoui and Cappé (2007). This penalty generalizes the one proposed by Lebarbier (2005) for a one-dimensional signal changing only through its mean. We prove a non-asymptotic oracle inequality for the proposed method, thanks to a new concentration result for some function of Hilbert-space valued random variables. Experiments on synthetic and real data illustrate the accuracy of our method, showing that it can detect changes in the whole distribution of data, even when the mean and variance are constant.

Joint work with Sylvain Arlot (Orsay) and Zaïd Harchaoui (Seattle). This work has been accepted in JMLR [15].

7.36. Axis 2: Analysis of early stopping rules based on discrepancy principle

Participant: Alain Celisse

We describe a general unified framework for analyzing the statistical performance of early stopping rules based on the minimum discrepancy principle (DP). Finite-sample bounds such as deviation or oracle inequalities are derived with high probability. Since it turns out that DP suffers some deficiencies when estimating smooth functions, refinements involving smoothing of the residuals are introduced and analyzed. Theoretical bounds established in the fixed design setting under mild assumptions such as the boundedness of the kernel. When focusing on the smoothed discrepancy principle, such bounds are even extended to the random design setting by means of a new change-of-norm argument

Joint work with Markus Reiß(Humboldt) and Martin Wahl (Humboldt). This work has been already presented several times in seminars.

7.37. Axis 3: Short-term air temperature forecasting using Nonparametric Functional Data Analysis and SARMA models

Participant: Sophie Dabo-Niang

Air temperature is a significant meteorological variable that affects social activities and economic sectors. In this paper, a non-parametric and a parametric approach are used to forecast hourly air temperature up to 24 h in advance. The former is a regression model in the Functional Data Analysis framework. The nonlinear regression operator is estimated using a kernel function. The smoothing parameter is obtained by a cross-validation procedure and used for the selection of the optimal number of closest curves. The other method applied is a Seasonal Autoregressive Moving Average (SARMA) model, the order of which is determined by the Bayesian Information Criterion. The obtained forecasts are combined using weights calculated based on the forecast errors. The results show that SARMA has a better performance for the first 6 forecasted hours, after which the Non-Parametric Functional Data Analysis (NPFDA) model provides superior results. Forecast pooling improves the accuracy of the forecasts.

It is a joint work with Stelian Curceac (Rothamsted Research, UK) Camille Ternynck (CERIM, Université de Lille) Taha B.M.J. Ouarda (INRS, Québec, Canada) Fateh Chebana (INRS, Québec, Canada). This work has been published in the journal Environmental Modelling and Software [18].

7.38. Axis 3: Mathematical Modeling and Study of Random or Deterministic Phenomena

Participant: Sophie Dabo-Niang

In order to identify mathematical modeling (including functional data analysis) and interdisciplinary research issues in evolutionary biology, epidemiology, epistemology, environmental and social sciences encountered by researchers in Mayotte, the first international conference on mathematical modeling (CIMOM'18) was held in Dembéni, Mayotte, from November 15 to 17, 2018, at the Centre Universitaire de Formation et de Recherche. The objective was to focus on mathematical research with interdisciplinarity. This contribution is a book discusses key aspects of recent developments in applied mathematical analysis and modeling. It was written after the international conference on mathematical modeling in Mayotte, where a call for chapters of the book was made. They were written in the form of journal articles, with new results extending the talks given during the conference and were reviewed by independent reviewers and book publishers It highlights a wide range of applications in the fields of biological and environmental sciences, epidemiology and social perspectives. Each chapter examines selected research problems and presents a balanced mix of theory and applications on some selected topics. Particular emphasis is placed on presenting the fundamental developments in mathematical analysis and modeling and highlighting the latest developments in different fields of probability and statistics. The chapters are presented independently and contain enough references to allow the reader to explore the various topics presented.

It is a joint work with Solym Manou-Abi and Jean-Jacques Salone (University of Mayotte, France). This book is to appear Wiley (ISTE) [21].

7.39. Axis 3: Categorical functional data analysis

Participants: Cristian Preda, Quentin Grimonprez, Vincent Vandewalle.

The research on functional data analysis is very actual. The R package "fda" is the most famous one implementing methodology for functional data. To the best of our knowledge, and quite surprisingly, there is no recent researches devoted to categorical functional data despite its ability to model real situations in different fields of applications: health and medicine (status of a patient over time), economy (status of the market), sociology (evolution of social status), and so on. We have developed the methodology to visualize, do dimension reduction and extract feature from categorical functional data. For this, the *cfda* R package has been developed.

7.40. Axis 4: Proteomic signature of early death in heart failure patients

Participants: Guillemette Marot, Vincent Vandewalle.

Heart failure (HF) remains a main cause of mortality worldwide. Risk stratification of patients with systolic chronic HF is critical to identify those who may benefit from advanced HF therapies. The aim of this study is to identify plasmatic proteins that could predict the early death (within 3 years) of HF patients with reduced ejection fraction hospitalized in CHRU de Lille. In this framework, we have performed LASSO logistic regression to perform variable selection in order to select candidates protein to predict early death in HF patients. An article has been accepted in Scientific Reports [19].

This is a joint work with Marie Cuvelliez, Florence Pinet and Christophe Bauters from INSERM.

7.41. Axis 4: Statistical analysis of high-throughput proteomic data

Participants: Guillemette Marot, Vincent Vandewalle, Wilfried Heyse.

From March until August 2019, Guillemette Marot and Vincent Vandewalle have supervised the internship of Wilfried Heyse (Master 2 Ingénieurie de Sytèmes Numériques). The purpose of this internship was to identify new circulating biomarkers of left ventricular remodelling (LVR) in patients suffering from myocardial infarction (MI). The aim is to precisely identify earlier after MI the patients at high risk of developing LVR that is quantified by imaging one year after MI. For that purpose, high throughput proteomic approach was used. This technology allows the measurement of 5000 proteins simultaneously. In parallel to these measures corresponding to the concentration of a protein in a plasma sample collected from one patient at a specific time, echocardiographic and clinical information will be collected on each of the 200 patients. Several approaches have been used to predict the LVR based on proteins measurements. In particular penalized regression such as LASSO and variable clustering. Wilfried Heyse has now started a Phd Thesis granted by INSERM and supervised by Christophe Bauters, Guillemette Marot and Vincent Vandewalle. One of the main challenge is to take into account the variations of the biomarkers according to the time (several measurement times), in order the improve the understanding of biological mechanisms involved on LVR.

This is a joint work with Florence Pinet and Christophe Bauters from INSERM.

7.42. Axis 4: Linking different kinds of Omics data through a model-based clustering approach

Participants: Guillemette Marot, Vincent Vandewalle, Wilfried Heyse.

In this work, a mixture model allowing for genes clustering using both microarray (continuous) and RNAseq (count) expression data is proposed. More generally, it answers the clustering of variables issue, when variables are of different kinds (continuous and discrete here). Variables describing the same gene are constrained to belong to the same cluster. This constraint allows us to obtain a model that links the microarray and RNAseq measurements without needing parametric constraints on the form of this link. The proposed approach has been illustrated on simulated data, as well as on real data from TCGA (The Cancer Genome Atlas). It has been presented in an international conference [49].

This is a joint work with Camille Ternynck from EA2694.

7.43. 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 published in an international journal [16] and Maxime Baelde defended his PhD thesis on this topic this year [11].

It is a joint work with Raphaël Greff, from the A-Volute company.

7.44. 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. Anne-Lise Bedenel defended her PhD thesis on this topic this year [12].

It is a joint work with Laetitia Jourdan, from Université de Lille.

7.45. 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. Adrien Ehrhardt defended his PhD thesis on this topic this year [13]. A preprint is being finalized to be submitted to an international journal or conference [62].

This is a joint work with Philippe Heinrich from Université de Lille.

7.46. 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 (for Mixmod,MixtComp and BlockCluster) directly in the web platform itself has led to some specific developments. In 2019, MASSICCC has been presented to a workshop [39]. In addition, the Mixtcomp software is now available on the CRAN depository. 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

7.47. Axis 4: Domain adaptation from a pre-trained source model

Participants: Christophe Biernacki, Pascal Germain, Luxin Zhang.

Traditional statistical learning paradigm assumes the consistency between train and test data distributions. This rarely holds in many real-life applications. The domain adaptation paradigm proposes a variety of techniques to overcome this issue. Most of the works in this area seek either for a latent space where source and target data share the same distribution, or for a transformation of the source distribution to match the target one. Both strategies require learning a model on the transformed source data. An original scenario is studied where one is given a model that has been constructed using expertise on the source data that is not accessible anymore. To use directly this model on target data, we propose to learn a transformation from the target domain to the source domain. Up to our knowledge, this is a new perspective on domain adaptation. This learning problem is introduced and formalized. We study the assumptions and the sufficient conditions mandatory to guarantee a good accuracy when using the source model directly on transformed target data. By pursuing this idea, a new domain adaptation method based on optimal transport is proposed. We experiment our method on a fraud detection problem.

Luxin Zhang begun his PhD thesis on this topic and presented this early result in an international conference [51].

It is a joint work with Yacine Kessaci, both from Worldline.

7.48. Axis 4: Reject Inference Methods in Credit Scoring: a rational review

Participants: Christophe Biernacki, Vincent Vandewalle, Adrien Ehrhardt.

The granting process of all credit institutions is based on the probability that the applicant will refund his/her loan given his/her characteristics. This probability also called score is learnt based on a dataset in which rejected applicants are de facto excluded. This implies that the population on which the score is used will be different from the learning population. Thus, this biased learning can have consequences on the scorecard's relevance. Many methods dubbed reject inference have been developed in order to try to exploit the data available from the rejected applicants to build the score. However most of these methods are considered from an empirical point of view, and there is some lack of formalization of the assumptions that are really made, and of the theoretical properties that can be expected. We propose a formalisation of these usually hidden assumptions for some of the most common reject inference methods, and we discuss the improvement that can be expected. These conclusions are illustrated on simulated data and on real data from Credit Agricole Consumer Finance (CACF), a major European loan issuer. Adrien Ehrhardt defended his PhD thesis on this topic this year [13]. A preprint is being finalized to be submitted to an international journal or conference.

This is a joint work with Philippe Heinrich from Université de Lille.

7.49. Other: 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 now under minor revision in an international journal [53].

It is a joint work with Hiba Alawieh and Nicolas Wicker, both from Université de Lille.

RANDOPT Project-Team

7. New Results

7.1. A multiobjective algorithm framework and the COMO-CMA-ES algorithm

One classical way to solve multiobjective optimization problems is to transform the multiple objective functions into a single one, also known as scalarization, and to solve multiple versions of such scalarizations to achieve multiple trade-off points. Another approach, coming from the field of evolutionary multiobjective optimization is to formulate a single-objective *set* problem via indicators: the goal here is to find the set of solutions (of a given size) that maximizes a certain quality. The hypervolume indicator has been regularly used to define the quality of the solution set because it has favorable theoretical properties.

The "classical" definition of the hypervolume indicator and how it is used in multiobjective solvers, however, has some disadvantages: (i) the resulting single-objective problem is of high dimension and the gradient of the hypervolume indicator is zero in dominated areas of the search space—not giving a solver enough information about where to search for good solutions. In [7], we discussed and visualized these disadvantages and proposed a new quality criterion which is based on the hypervolume indicator but solves the mentioned disadvantages. The implementation of this idea and its combination with the single-objective solver CMA-ES resulted in the COMO-CMA-ES which shows improved performance over several existing multiobjective solvers on a wide range of convex quadratic functions.

7.2. A mixed-integer benchmark testbed for single and multiobjective black-box optimization

We have introduced two suites of mixed-integer benchmark problems to be used for analyzing and comparing black-box optimization algorithms. They contain problems of diverse difficulties that are scalable in the number of decision variables. The bbob-mixint suite is designed by partially discretizing the established BBOB (Black-Box Optimization Benchmarking) problems. The bi-objective problems from the bbob-biobj-mixint suite are, on the other hand, constructed by using the bbob-mixint functions as their separate objectives. We explain the rationale behind our design decisions and show how to use the suites within the COCO (Comparing Continuous Optimizers) platform. Analyzing two chosen functions in more detail, we also provide some unexpected findings about their properties [8].

7.3. A large-scale optimization testbed for the COCO framework

We have finalized a large scale testbed built to model well-known difficulties in continuous optimization and to test the scaling behavior of algorithms. It contrasts with current test suites used for benchmarking solvers.

The test suite contains 24 single-objective functions in continuous domain and extends the well-known single-objective noiseless bbob test suite. A core contribution is to reduce the computational demand of the orthogonal search space transformations, that appear in the bbob test suite, while retaining some desired properties using previously introduced permuted block diagonal orthogonal matrices.

The paper discusses the implementation details, particularly the normalization and scaling to obtain backwards compatibility with the bbob test suite. Additionally, a guide for using the test suite within the COCO platform, as well as a description of the postprocessed output is presented [12].

7.4. Diagonal Acceleration for Covariance Matrix Adaptation Evolution Strategies

In [1], we have introduced an acceleration for the covariance matrix adaptation evolution strategies (CMA-ES) by means of adaptive diagonal decoding (dd-CMA). This diagonal acceleration endows the default CMA-ES with the advantages of separable CMA-ES without inheriting its drawbacks. Technically, we introduce a diagonal matrix that expresses coordinate-wise variances of the sampling distribution. The diagonal matrix can learn a rescaling of the problem in the coordinates within linear number of function evaluations. Diagonal decoding can also exploit separability of the problem, but, crucially, does not compromise the performance on non-separable problems. The latter is accomplished by modulating the learning rate for the diagonal matrix based on the condition number of the underlying correlation matrix. dd-CMA-ES not only combines the advantages of default and separable CMA-ES, but may achieve overadditive speedup: it improves the performance, and even the scaling, of the better of default and separable CMA-ES on classes of non-separable test functions that reflect, arguably, a landscape feature commonly observed in practice. The paper makes two further secondary contributions: we introduce two different approaches to guarantee positive definiteness of the covariance matrix with active CMA, which is valuable in particular with large population size; we revise the default parameter setting in CMA-ES, proposing accelerated settings in particular for large dimension. All our contributions can be viewed as independent improvements of CMA-ES, yet they are also complementary and can be seamlessly combined. In numerical experiments with dd-CMA-ES up to dimension 5120, we observe remarkable improvements over the original covariance matrix adaptation on functions with coordinate-wise ill-conditioning. The improvement is observed also for large population sizes up to about dimension squared.

7.5. A global surrogate assisted CMA-ES

In the paper [5], we have explored the arguably simplest way to build an effective surrogate fitness model in continuous search spaces. The model complexity is linear or diagonal-quadratic or full quadratic, depending on the number of available data. The model parameters are computed from the Moore-Penrose pseudoinverse. The model is used as a surrogate fitness for CMA-ES if the rank correlation between true fitness and surrogate value of recently sampled data points is high. Otherwise, further samples from the current population are successively added as data to the model. We empirically compare the IPOP scheme of the new model assisted lq-CMA-ES with a variety of previously proposed methods and with a simple portfolio algorithm using SLSQP and CMA-ES. We conclude that a global quadratic model and a simple portfolio algorithm are viable options to enhance CMA-ES. The model building code is available as part of the pycma Python module on Github and PyPI.

7.6. Benchmarking and Understanding Optimizers

Benchmarking is an important task in optimization in order to understand the working principles behind existing solvers, to find out about weaknesses of them and to finally recommend good ones. The COCO platform, developed in the Randopt team since 2007, aims at automatizing these numerical benchmarking experiments and the visual presentation of their results. We regularly use the platform to initiate workshop papers during the ACM-GECCO conference and also held a workshop this year [0].

In this context, several workshop papers have been published by members of the team and we also proposed some extensions of the platform and updated its documentation.

Two papers addressed single-objective unconstrained problems. One paper investigated the impact of the sample volume of a simple random search on the bbob test suite of COCO [2] and the other paper benchmarked all solvers available in the scipy.optimize module of Python [9], re-discovering SLSQP as a very well-performing solver for small budgets.

[0] See numbbo.github.io/workshops/BBOB-2019/

Two additional papers addressed multiobjective problems in the context of the bbob-biobj test suite of COCO: “Benchmarking Algorithms from the platypus Framework on the Biobjective bbob-biobj Testbed” [3] compared several baseline algorithms from the literature such as NSGA-II, MOEA/D, SPEA2, and IBEA and “Benchmarking MO-CMA-ES and COMO-CMA-ES on the Bi-objective bbob-biobj Testbed” [4] compared our new COMO-CMA-ES solver with its previous version MO-CMA-ES.

As to extensions of the COCO platform, we released new test suites this year as described earlier. For the large-scale test suite of [12], 11 algorithm variants of the CMA-ES and L-BFGS solvers have been compared in the paper “Benchmarking Large Scale Variants of CMA-ES and L-BFGS-B on the bbob-largescale Testbed” [10].

Overall, we collected 54 new algorithm data sets within the COCO platform in 2019—the highest number in a single year since the release of COCO.

Finally, we updated our documentation on the biobjective test suite, we introduced in 2019. The corresponding journal paper “Using Well-Understood Single-Objective Functions in Multiobjective Black-Box Optimization Test Suites” [11] is now under revision for the Evolutionary Computation journal.

REALOPT Project-Team

7. New Results

7.1. An iterative dynamic programming approach for the temporal knapsack problem

We have developed an approach to solve the temporal knapsack problem (TKP) based on a very large size dynamic programming formulation [28]. In this generalization of the classical knapsack problem, selected items enter and leave the knapsack at fixed dates. We solve the TKP with a dynamic program of exponential size, which is solved using a method called Successive Sublimation Dynamic Programming (SSDP). This method starts by relaxing a set of constraints from the initial problem, and iteratively reintroduces them when needed. We show that a direct application of SSDP to the temporal knapsack problem does not lead to an effective method, and that several improvements are needed to compete with the best results from the literature.

7.2. A Hypergraph Model for the Rolling Stock Rotation Planning and Train Selection Problem

We investigated an integrated optimization approach for timetabling and rolling stock rotation planning in the context of passenger railway traffic [27]. Given a set of possible passenger trips, service requirement constraints, and a fleet of multiple heterogeneous self-powered railcars, our method aims at producing a timetable and solving the rolling stock problem in such a way that the use of railcars and the operational costs are minimized. To solve this hard optimization problem, we design a mixed-integer linear programming model based on network-flow in an hypergraph. We use this models to handle effectively constraints related to coupling and decoupling railcars. To reduce the size of the model, we use an aggregation and disaggregation technique combined with reduced-cost filtering. Computational experiments based on several French regional railway traffic case studies show that our method scales successfully to real-life problems.

7.3. Decomposition-based approaches for a class of two-stage robust binary optimization problems

We have studied a class of two-stage robust binary optimization problems with objective uncertainty where recourse decisions are restricted to be mixed-binary [25]. For these problems, we present a deterministic equivalent formulation through the convexification of the recourse feasible region. We then explore this formulation under the lens of a relaxation, showing that the specific relaxation we propose can be solved using the branch-and-price algorithm. We present conditions under which this relaxation is exact, and describe alternative exact solution methods when this is not the case. Despite the two-stage nature of the problem, we provide NP-completeness results based on our reformulations. Finally, we present various applications in which the methodology we propose can be applied. We compare our exact methodology to those approximate methods recently proposed in the literature under the name K-adaptability. Our computational results show that our methodology is able to produce better solutions in less computational time compared to the K-adaptability approach, as well as to solve bigger instances than those previously managed in the literature.

7.4. Primal heuristic for Branch-and-Price

Primal heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending MIP based heuristics, our study outlines generic procedures to build primal solutions in the context of a branch-and-price approach and reports on their performance. Our heuristic decisions carry on variables of the Dantzig-Wolfe reformulation, the motivation being to take advantage of a tighter linear programming relaxation than that of the original compact formulation and to benefit from the combinatorial structure embedded in these variables. In [9], we focus on the so-called diving methods that use re-optimization after each LP rounding. We explore combinations with diversification-intensification paradigms such as limited discrepancy search, sub-MIPing, 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.

7.5. Generic solver for vehicle routing problems

Major advances were recently obtained in the exact solution of Vehicle Routing Problems (VRPs). Sophisticated Branch-Cut-and-Price (BCP) algorithms for some of the most classical VRP variants now solve many instances with up to a few hundreds of customers. However, adapting and re-implementing those successful algorithms for other variants can be a very demanding task. In [8], [12], [11], we propose a BCP solver for a generic model that encompasses a wide class of VRPs. It incorporates the key elements found in the best existing VRP algorithms: ng-path relaxation, rank-1 cuts with limited memory, path enumeration, and rounded capacity cuts; all generalized through the new concepts of “packing set” and “elementarity set”. The concepts are also used to derive a branching rule based on accumulated resource consumption and to generalize the Ryan and Foster branching rule. Extensive experiments on several variants show that the generic solver has an excellent overall performance, in many problems being better than the best specific algorithms. Even some non-VRPs, like bin packing, vector packing and generalized assignment, can be modeled and effectively solved.

The solver is available for download and free academic use in http://vrpsolver.math.u-bordeaux.fr.

7.6. New algorithms for different vehicle routing problems

In [7], we propose a branch-cut-and-price algorithm for the two-echelon capacitated vehicle routing problem in which delivery of products from a depot to customers is performed using intermediate depots called satellites. We introduce a new route based formulation for the problem which does not use variables to determine product flows in satellites. Second, we introduce a new branching strategy which significantly decreases the size of the branch-and-bound tree. Third, we introduce a new family of satellite supply inequalities, and we empirically show that it improves the quality of the dual bound at the root node of the branch-and-bound tree. Finally, extensive numerical experiments reveal that our algorithm can solve to optimality all literature instances with up to 200 customers and 10 satellites for the first time and thus double the size of instances which could be solved to optimality.

In [22], [21], we are interested in the exact solution of the vehicle routing problem with backhauls (VRPB), a classical vehicle routing variant with two types of customers: linehaul (delivery) and backhaul (pickup) ones. We propose two branch-cut-and-price (BCP) algorithms for the VRPB. The first of them follows the traditional approach with one pricing subproblem, whereas the second one exploits the linehaul/backhaul customer partitioning and defines two pricing subproblems. The methods incorporate elements of state-of-the-art BCP algorithms, such as rounded capacity cuts, limited-memory rank-1 cuts, strong branching, route enumeration, arc elimination using reduced costs and dual stabilization. Computational experiments show that the proposed algorithms are capable of obtaining optimal solutions for all existing benchmark instances with up to 200 customers, many of them for the first time. It is observed that the approach involving two pricing subproblems is more efficient computationally than the traditional one. Moreover, new instances are also proposed for which we provide tight bounds. Also, we provide results for benchmark instances of the heterogeneous fixed fleet VRPB and the VRPB with time windows.

In [20], we consider the standard Capacitated Location-Routing Problem (LRP), which is the combination of two canonical combinatorial optimization problems : Facility Location Problem (FLP), and Vehicle Routing Problem (VRP). We have extended the Branch-and-Cut-and-Price Algorithm from [11] to solve a Mixed

Integer Programming (MIP) formulation with and exponential number of varialbes. A new family of Route Load Knapsack valid inequalites is proposed to strengthen the formulation. Preliminary results showed that our algorithm could solve to optimality, for the first time, 12 open instances of the most difficult classes of LRP instances.

In the first echelon of the two-echelon stochastic multi-period capacitated location-routing problem (2E-SM-CLRP), one has to decide the number and location of warehouse platforms as well as the intermediate distribution platforms for each period; while fixing the capacity of the links between them. The system must be dimensioned to enable an efficient distribution of goods to customers under a stochastic and time-varying demand. In the second echelon of the 2E-SM-CLRP, the goal is to construct vehicle routes that visit customers from operating distribution platforms. The objective is to minimize the total expected cost. We model this hierarchical decision problem as a two-stage stochastic program with integer recourse. The first-stage includes location and capacity decisions to be fixed at each period over the planning horizon, while routing decisions of the second echelon are determined in the recourse problem. In [16], [26], we propose a Benders decomposition approach to solve this model. In the proposed approach, the location and capacity decisions are taken by solving the Benders master problem. After these first-stage decisions are fixed, the resulting subproblem is a capacitated vehicle-routing problem with capacitated multi-depot (CVRP-CMD) that is solved by a branch-cut-and-price algorithm. Computational experiments show that instances of realistic size can be solved optimally within reasonable time, and that relevant managerial insights are derived on the behavior of the design decisions under the stochastic multi-period characterization of the planning horizon.

Much of the existing research on electric vehicle routing problems (E-VRPs) assumes that the charging stations (CSs) can simultaneously charge an unlimited number of electric vehicles, but this is not the case. In [29], we investigate how to model and solve E-VRPs taking into account these capacity restrictions. In particular, we study an E-VRP with non-linear charging functions, multiple charging technologies, en route charging, and variable charging quantities, while explicitly accounting for the capacity of CSs expressed in the number of chargers. We refer to this problem as the E-VRP with non-linear charging functions and capacitated stations (E-VRP-NL-C). This problem advances the E-VRP literature by considering the scheduling of charging operations at each CS. We first introduce two mixed integer linear programming formulations showing how CS capacity constraints can be incorporated into E-VRP models. We then introduce an algorithmic framework to the E-VRP-NL-C, that iterates between two main components: a route generator and a solution assembler. The route generator uses an iterated local search algorithm to build a pool of high-quality routes. The solution assembler applies a branch-and-cut algorithm to select a subset of routes from the pool. We report on computational experiments comparing four different assembly strategies on a large and diverse set of instances. Our results show that our algorithm deals with the CS capacity constraints effectively. Furthermore, considering the well-known uncapacitated version of the E-VRP-NL-C, our solution method identifies new best-known solutions for 80 out of 120 instances.

7.7. Packing problems

In the two-dimensional guillotine cutting-stock problem, the objective is to minimize the number of large plates used to cut a list of small rectangles. We consider a variant of this problem, which arises in glass industry when different bills of order (or batches) are considered consecutively. For practical organisation reasons, leftovers are not reused, except the large one obtained in the last cutting pattern of a batch, which can be reused for the next batch. The problem can be decomposed into an independent problem for each batch. In [6] we focus on the one-batch problem, the objective of which is to minimize the total width of the cutting patterns used. We propose a diving heuristic based on 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 strengthens the lower bounds obtained by column generation and improves the quality of the 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 glass industry data. According to these results, variants of the proposed diving heuristic outperform constructive and evolutionary heuristics.instances than those previously managed in the literature.

The bin packing problem with generalized time lags (BPGL) consists of a set of items, each having a positive weight, and a set of precedence constraints with lags between pairs of items, allowing negative and non-negative lags. The items must be packed into the minimum possible number of bins with identical capacity, and the bins must be assigned to time periods satisfying the precedence constraints with lags on the items. In [18] we show a solution strategy using a generic branch-and-price algorithm (implemented in the software platform BaPCod) and applying some problem specific cuts. Our approach outperformed the compact Mixed Integer Programming (MIP) formulation solved by the MIP solver Cplex.

7.8. Covering problems

In [5], we study a covering problem where vertices of a graph have to be covered by rooted sub-trees. We present three mixed-integer linear programming models, two of which are compact while the other is based on Dantzig-Wolfe decomposition. In the latter case, we focus on the column generation sub-problem, a knapsack problem with precedence constraints on trees, for which we propose several algorithms among them a branch and bound algorithm and various dynamic programs. Numerical results are obtained using instances from the literature and instances based on a real-life districting application. Experiments show that the branch-and-price algorithm is able to solve much bigger instances than the compact model, which is limited to very small instance sizes.

7.9. Software Defined Networking

ISP networks are taking a leap forward thanks to emerging technologies such as Software Defined Networking (SDN) and Network Function Virtualization (NFV). Efficient algorithms considered too hard to be put in practice on legacy networks now have a second chance to be considered again. In this context, we rethink the ISP network dimensioning problem with protection against Shared Risk Link Group (SLRG) failures. In [30], [15], [23], we consider a path-based protection scheme with a global rerouting strategy, in which, for each failure situation, we may have a new routing of all the demands. Our optimization task is to minimize the needed amount of bandwidth. After discussing the hardness of the problem, we develop two scalable mathematical models that we handle using both Column Generation and Benders Decomposition techniques. Through extensive simulations on real-world IP network topologies and on random generated instances, we show the effectiveness of our methods. Finally, our implementation in OpenDaylight demonstrates the feasibility of the approach and its evaluation with Mininet shows that technical implementation choices may have a dramatic impact on the time needed to reestablish the flows after a failure takes place.

SEQUEL Project-Team

7. New Results

7.1. Decision-making Under Uncertainty

7.1.1. Reinforcement Learning

Model-Based Reinforcement Learning Exploiting State-Action Equivalence, [16]

Leveraging an equivalence property in the state-space of a Markov Decision Process (MDP) has been investigated in several studies. This paper studies equivalence structure in the reinforcement learning (RL) setup, where transition distributions are no longer assumed to be known. We present a notion of similarity between transition probabilities of various state-action pairs of an MDP, which naturally defines an equivalence structure in the state-action space. We present equivalence-aware confidence sets for the case where the learner knows the underlying structure in advance. These sets are provably smaller than their corresponding equivalence-oblivious counterparts. In the more challenging case of an unknown equivalence structure, we present an algorithm called ApproxEquivalence that seeks to find an (approximate) equivalence structure, and define confidence sets using the approximate equivalence. To illustrate the efficacy of the presented confidence sets, we present C-UCRL, as a natural modification of UCRL2 for RL in undiscounted MDPs. In the case of a known equivalence structure, we show that C-UCRL improves over UCRL2 in terms of regret by a factor of SA/C, in any communicating MDP with S states, A actions, and C classes, which corresponds to a massive improvement when C SA. To the best of our knowledge, this is the first work providing regret bounds for RL when an equivalence structure in the MDP is efficiently exploited. In the case of an unknown equivalence structure, we show through numerical experiments that C-UCRL combined with ApproxEquivalence outperforms UCRL2 in ergodic MDPs.

Practical Open-Loop Optimistic Planning, [25]

We consider the problem of online planning in a Markov Decision Process when given only access to a generative model, restricted to open-loop policies-i.e. sequences of actions-and under budget constraint. In this setting, the Open-Loop Optimistic Planning (OLOP) algorithm enjoys good theoretical guarantees but is overly conservative in practice, as we show in numerical experiments. We propose a modified version of the algorithm with tighter upper-confidence bounds, KL-OLOP, that leads to better practical performances while retaining the sample complexity bound. Finally, we propose an efficient implementation that significantly improves the time complexity of both algorithms.

Budgeted Reinforcement Learning in Continuous State Space, [20]

A Budgeted Markov Decision Process (BMDP) is an extension of a Markov Decision Process to critical applications requiring safety constraints. It relies on a notion of risk implemented in the shape of a cost signal constrained to lie below an-adjustable-threshold. So far, BMDPs could only be solved in the case of finite state spaces with known dynamics. This work extends the state-of-the-art to continuous spaces environments and unknown dynamics. We show that the solution to a BMDP is a fixed point of a novel Budgeted Bellman Optimality operator. This observation allows us to introduce natural extensions of Deep Reinforcement Learning algorithms to address large-scale BMDPs. We validate our approach on two simulated applications: spoken dialogue and autonomous driving.

Regret Bounds for Learning State Representations in Reinforcement Learning, [29]

We consider the problem of online reinforcement learning when several state representations (mapping histories to a discrete state space) are available to the learning agent. At least one of these representations is assumed to induce a Markov decision process (MDP), and the performance of the agent is measured in terms of cumulative regret against the optimal policy giving the highest average reward in this MDP representation. We propose an algorithm (UCB-MS) with O($\sqrt{T}$) regret in any communicating MDP. The regret bound shows that UCB-MS automatically adapts to the Markov model and improves over the currently known best bound of order O(T 2/3).

Planning in entropy-regularized Markov decision processes and games, [24]

We propose SmoothCruiser, a new planning algorithm for estimating the value function in entropy-regularized Markov decision processes and two-player games, given a generative model of the environment. SmoothCruiser makes use of the smoothness of the Bellman operator promoted by the regularization to achieve problem-independent sample complexity of order O(1/ϵ 4) for a desired accuracy ϵ, whereas for non-regularized settings there are no known algorithms with guaranteed polynomial sample complexity in the worst case.

7.1.1.1. Deep reinforcement learning

"I'm sorry Dave, I'm afraid I can't do that" Deep Q-Learning From Forbidden Actions, [42]

The use of Reinforcement Learning (RL) is still restricted to simulation or to enhance human-operated systems through recommendations. Real-world environments (e.g. industrial robots or power grids) are generally designed with safety constraints in mind implemented in the shape of valid actions masks or contingency controllers. For example, the range of motion and the angles of the motors of a robot can be limited to physical boundaries. Violating constraints thus results in rejected actions or entering in a safe mode driven by an external controller, making RL agents incapable of learning from their mistakes. In this paper, we propose a simple modification of a state-of-the-art deep RL algorithm (DQN), enabling learning from forbidden actions. To do so, the standard Q-learning update is enhanced with an extra safety loss inspired by structured classification. We empirically show that it reduces the number of hit constraints during the learning phase and accelerates convergence to near-optimal policies compared to using standard DQN. Experiments are done on a Visual Grid World Environment and Text-World domain.

MERL: Multi-Head Reinforcement Learning, [39]

A common challenge in reinforcement learning is how to convert the agent's interactions with an environment into fast and robust learning. For instance, earlier work makes use of domain knowledge to improve existing reinforcement learning algorithms in complex tasks. While promising, previously acquired knowledge is often costly and challenging to scale up. Instead, we decide to consider problem knowledge with signals from quantities relevant to solve any task, e.g., self-performance assessment and accurate expectations. $\mathcal{V}^{ex}$ is such a quantity. It is the fraction of variance explained by the value function V and measures the discrepancy between V and the returns. Taking advantage of $\mathcal{V}^{ex}$, we propose MERL, a general framework for structuring reinforcement learning by injecting problem knowledge into policy gradient updates. As a result, the agent is not only optimized for a reward but learns using problem-focused quantities provided by MERL, applicable out-of-the-box to any task. In this paper: (a) We introduce and define MERL, the multi-head reinforcement learning framework we use throughout this work. (b) We conduct experiments across a variety of standard benchmark environments, including 9 continuous control tasks, where results show improved performance. (c) We demonstrate that MERL also improves transfer learning on a set of challenging pixel-based tasks. (d) We ponder how MERL tackles the problem of reward sparsity and better conditions the feature space of reinforcement learning agents.

Self-Educated Language Agent With Hindsight Experience Replay For Instruction Following, [45]

Language creates a compact representation of the world and allows the description of unlimited situations and objectives through compositionality. These properties make it a natural fit to guide the training of interactive agents as it could ease recurrent challenges in Reinforcement Learning such as sample complexity, generalization, or multi-tasking. Yet, it remains an open-problem to relate language and RL in even simple instruction following scenarios. Current methods rely on expert demonstrations, auxiliary losses, or inductive biases in neural architectures. In this paper, we propose an orthogonal approach called Textual Hindsight Experience Replay (THER) that extends the Hindsight Experience Replay approach to the language setting. Whenever the agent does not fulfill its instruction, THER learns to output a new directive that matches the agent trajectory, and it relabels the episode with a positive reward. To do so, THER learns to map a state into an instruction by using past successful trajectories, which removes the need to have external expert interventions to relabel episodes as in vanilla HER. We observe that this simple idea also initiates a learning synergy between language acquisition and policy learning on instruction following tasks in the BabyAI environment.

High-Dimensional Control Using Generalized Auxiliary Tasks, [47]

A long-standing challenge in reinforcement learning is the design of function approximations and efficient learning algorithms that provide agents with fast training, robust learning, and high performance in complex environments. To this end, the use of prior knowledge, while promising, is often costly and, in essence, challenging to scale up. In contrast, we consider problem knowledge signals, that are any relevant indicator useful to solve a task, e.g., metrics of uncertainty or proactive prediction of future states. Our framework consists of predicting such complementary quantities associated with self-performance assessment and accurate expectations. Therefore, policy and value functions are no longer only optimized for a reward but are learned using environment-agnostic quantities. We propose a generally applicable framework for structuring reinforcement learning by injecting problem knowledge in policy gradient updates. In this paper: (a) We introduce MERL, our multi-head reinforcement learning framework for generalized auxiliary tasks. (b) We conduct experiments across a variety of standard benchmark environments. Our results show that MERL improves performance for on- and off-policy methods. (c) We show that MERL also improves transfer learning on a set of challenging tasks. (d) We investigate how our approach addresses the problem of reward sparsity and pushes the function approximations into a better-constrained parameter configuration.

7.1.2. Multi-armed Bandit Theory

Asymptotically Optimal Algorithms for Budgeted Multiple Play Bandits, [15]

We study a generalization of the multi-armed bandit problem with multiple plays where there is a cost associated with pulling each arm and the agent has a budget at each time that dictates how much she can expect to spend. We derive an asymptotic regret lower bound for any uniformly efficient algorithm in our setting. We then study a variant of Thompson sampling for Bernoulli rewards and a variant of KL-UCB for both single-parameter exponential families and bounded, finitely supported rewards. We show these algorithms are asymptotically optimal, both in rateand leading problem-dependent constants, including in the thick margin setting where multiple arms fall on the decision boundary.

Non-Asymptotic Pure Exploration by Solving Games, [46]

Pure exploration (aka active testing) is the fundamental task of sequentially gathering information to answer a query about a stochastic environment. Good algorithms make few mistakes and take few samples. Lower bounds (for multi-armed bandit models with arms in an exponential family) reveal that the sample complexity is determined by the solution to an optimisation problem. The existing state of the art algorithms achieve asymptotic optimality by solving a plug-in estimate of that optimisation problem at each step. We interpret the optimisation problem as an unknown game, and propose sampling rules based on iterative strategies to estimate and converge to its saddle point. We apply no-regret learners to obtain the first finite confidence guarantees that are adapted to the exponential family and which apply to any pure exploration query and bandit structure. Moreover, our algorithms only use a best response oracle instead of fully solving the optimisation problem.

Rotting bandits are not harder than stochastic ones, [32]

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, O(log(KT)), and problem-independent, O($sqrtKT$), 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 O(K1/3T2/3). Finally, we report simulations confirming the theoretical improvements of FEWA.

7.1.3. Black-box Optimization

General parallel optimization without a metric, [34]

Hierarchical bandits are 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. On top of that, we propose a general wrapper, called GPO, that can cope with algorithms that only have simple regret guarantees. Finally, we complement our findings with experiments on difficult functions.

A simple dynamic bandit algorithm for hyper-parameter tuning, [33]

Hyper-parameter tuning is a major part of modern machine learning systems. The tuning itself can be seen as a sequential resource allocation problem. As such, methods for multi-armed bandits have been already applied. In this paper, we view hyper-parameter optimization as an instance of best-arm identification in infinitely many-armed bandits. We propose D-TTTS, a new adaptive algorithm inspired by Thompson sampling, which dynamically balances between refining the estimate of the quality of hyper-parameter configurations previously explored and adding new hyper-parameter configurations to the pool of candidates. The algorithm is easy to implement and shows competitive performance compared to state-of-the-art algorithms for hyper-parameter tuning.

7.1.4. Statistics for Machine Learning

Non-asymptotic analysis of a sequential rupture detection test and its application to non-stationary bandits, [36]

We study a strategy for online change-point detection based on generalized likelihood ratios (GLR) and that can be expressed with the binary relative entropy. This test is used to detect a change in the mean of a bounded distribution, and we propose a non-asymptotic control of its false alarm probability and detection delay. We then explain how it can be useful for sequential decision making by proposing the GLR-klUCB bandit strategy, which is efficient in piece-wise stationary multi-armed bandit models.

Sequential change-point detection: Laplace concentration of scan statistics and non-asymptotic delay bounds, [27]

We consider change-point detection in a fully sequential setup, when observations are received one by one and one must raise an alarm as early as possible after any change. We assume that both the change points and the distributions before and after the change are unknown. We consider the class of piecewise-constant mean processes with sub-Gaussian noise, and we target a detection strategy that is uniformly good on this class (this constrains the false alarm rate and detection delay). We introduce a novel tuning of the GLR test that takes here a simple form involving scan statistics, based on a novel sharp concentration inequality using an extension of the Laplace method for scan-statistics that holds doubly-uniformly in time. This also considerably simplifies the implementation of the test and analysis. We provide (perhaps surprisingly) the first fully non-asymptotic analysis of the detection delay of this test that matches the known existing asymptotic orders, with fully explicit numerical constants. Then, we extend this analysis to allow some changes that are not-detectable by any uniformly-good strategy (the number of observations before and after the change are too small for it to be detected by any such algorithm), and provide the first robust, finite-time analysis of the detection delay.

Learning Multiple Markov Chains via Adaptive Allocation, [35]

We study the problem of learning the transition matrices of a set of Markov chains from a single stream of observations on each chain. We assume that the Markov chains are ergodic but otherwise unknown. The learner can sample Markov chains sequentially to observe their states. The goal of the learner is to sequentially select various chains to learn transition matrices uniformly well with respect to some loss function. We introduce a notion of loss that naturally extends the squared loss for learning distributions to the case of Markov chains, and further characterize the notion of being uniformly good in all problem instances. We present a novel learning algorithm that efficiently balances exploration and exploitation intrinsic to this problem, without any prior knowledge of the chains. We provide finite-sample PAC-type guarantees on the performance of the algorithm. Further, we show that our algorithm asymptotically attains an optimal loss.

7.1.5. DPP

On two ways to use determinantal point processes for Monte Carlo integration, [40]

This paper focuses on Monte Carlo integration with determinantal point processes (DPPs) which enforce negative dependence between quadrature nodes. We survey the properties of two unbiased Monte Carlo estimators of the integral of interest: a direct one proposed by Bardenet & Hardy (2016) and a less obvious 60-year-old estimator by Ermakov & Zolotukhin (1960) that actually also relies on DPPs. We provide an efficient implementation to sample exactly a particular multidimen-sional DPP called multivariate Jacobi ensemble. This let us investigate the behavior of both estima-tors on toy problems in yet unexplored regimes.

7.2. Applications

7.2.1. Autonomous car

Practical Open-Loop Optimistic Planning, [25]

We consider the problem of online planning in a Markov Decision Process when given only access to a generative model, restricted to open-loop policies-i.e. sequences of actions-and under budget constraint. In this setting, the Open-Loop Optimistic Planning (OLOP) algorithm enjoys good theoretical guarantees but is overly conservative in practice, as we show in numerical experiments. We propose a modified version of the algorithm with tighter upper-confidence bounds, KL-OLOP, that leads to better practical performances while retaining the sample complexity bound. Finally, we propose an efficient implementation that significantly improves the time complexity of both algorithms.

Budgeted Reinforcement Learning in Continuous State Space, [20]

A Budgeted Markov Decision Process (BMDP) is an extension of a Markov Decision Process to critical applications requiring safety constraints. It relies on a notion of risk implemented in the shape of a cost signal constrained to lie below an-adjustable-threshold. So far, BMDPs could only be solved in the case of finite state spaces with known dynamics. This work extends the state-of-the-art to continuous spaces environments and unknown dynamics. We show that the solution to a BMDP is a fixed point of a novel Budgeted Bellman Optimality operator. This observation allows us to introduce natural extensions of Deep Reinforcement Learning algorithms to address large-scale BMDPs. We validate our approach on two simulated applications: spoken dialogue and autonomous driving.

7.2.2. Cognitive radio

Decentralized Spectrum Learning for IoT Wireless Networks Collision Mitigation, [28]

This paper describes the principles and implementation results of reinforcement learning algorithms on IoT devices for radio collision mitigation in ISM unlicensed bands. Learning is here used to improve both the IoT network capability to support a larger number of objects as well as the autonomy of IoT devices. We first illustrate the efficiency of the proposed approach in a proof-of-concept based on USRP software radio platforms operating on real radio signals. It shows how collisions with other RF signals present in the ISM band are diminished for a given IoT device. Then we describe the first implementation of learning algorithms on LoRa devices operating in a real LoRaWAN network, that we named IoTligent. The proposed solution adds neither processing overhead so that it can be ran in the IoT devices, nor network overhead so that no change is required to LoRaWAN. Real life experiments have been done in a realistic LoRa network and they show that IoTligent device battery life can be extended by a factor 2 in the scenarios we faced during our experiment.

GNU Radio Implementation of MALIN: "Multi-Armed bandits Learning for Internet-of-things Networks", [37]

We implement an IoT network in the following way: one gateway, one or several intelligent (i.e., learning) objects, embedding the proposed solution, and a traffic generator that emulates radio interferences from many other objects. Intelligent objects communicate with the gateway with a wireless ALOHA-based protocol, which does not require any specific overhead for the learning. We model the network access as a discrete sequential decision making problem, and using the framework and algorithms from Multi-Armed Bandit (MAB) learning, we show that intelligent objects can improve their access to the network by using low complexity and decentralized algorithms, such as UCB1 and Thompson Sampling. This solution could be added in a straightforward and costless manner in LoRaWAN networks, just by adding this feature in some or all the devices, without any modification on the network side.

7.2.3. Other

Accurate reconstruction of EBSD datasets by a multimodal data approach using an evolutionary algorithm, [14]

A new method has been developed for the correction of the distortions and/or enhanced phase differentiation in Electron Backscatter Diffraction (EBSD) data. Using a multi-modal data approach, the method uses segmented images of the phase of interest (laths, precipitates, voids, inclusions) on images gathered by backscattered or secondary electrons of the same area as the EBSD map. The proposed approach then search for the best transformation to correct their relative distortions and recombines the data in a new EBSD file. Speckles of the features of interest are first segmented in both the EBSD and image data modes. The speckle extracted from the EBSD data is then meshed, and the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is implemented to distort the mesh until the speckles superimpose. The quality of the matching is quantified via a score that is linked to the number of overlapping pixels in the speckles. The locations of the points of the distorted mesh are compared to those of the initial positions to create pairs of matching points that are used to calculate the polynomial function that describes the distortion the best. This function is then applied to un-distort the EBSD data, and the phase information is inferred using the data of the segmented speckle. Fast and versatile, this method does not require any human annotation and can be applied to large datasets and wide areas. Besides, this method requires very few assumptions concerning the shape of the distortion function. It can be used for the single compensation of the distortions or combined with the phase differentiation. The accuracy of this method is of the order of the pixel size. Some application examples in multiphase materials with feature sizes down to 1 μm are presented, including Ti-6Al-4V Titanium alloy, Rene 65 and additive manufactured Inconel 718 Nickel-base superalloys.

Energy Management for Microgrids: a Reinforcement Learning Approach, [41]

This paper presents a framework based on reinforcement learning for energy management and economic dispatch of an islanded microgrid without any forecasting module. The architecture of the algorithm is divided in two parts: a learning phase trained by a reinforcement learning (RL) algorithm on a small dataset and the testing phase based on a decision tree induced from the trained RL. An advantage of this approach is to create an autonomous agent, able to react in real-time, considering only the past. This framework was tested on real data acquired at Ecole Polytechnique in France over a long period of time, with a large diversity in the type of days considered. It showed near optimal, efficient and stable results in each situation.

SIERRA Project-Team

7. New Results

7.1. Fast Gradient Methods for Symmetric Nonnegative Matrix Factorization.

We describe fast gradient methods for solving the symmetric nonnegative matrix factorization problem (SymNMF). We use recent results on non-Euclidean gradient methods and show that the SymNMF problem is smooth relative to a well-chosen Bregman divergence. This approach provides a simple hyperparameter-free method which comes with theoretical convergence guarantees. We also discuss accelerated variants. Numerical experiments on clustering problems show that our algorithm scales well and reaches both state of the art convergence speed and clustering accuracy for SymNMF methods.

7.2. Naive Feature Selection: Sparsity in Naive Bayes.

Due to its linear complexity, naive Bayes classification remains an attractive supervised learning method, especially in very large-scale settings. We propose a sparse version of naive Bayes, which can be used for feature selection. This leads to a combinatorial maximum-likelihood problem, for which we provide an exact solution in the case of binary data, or a bound in the multinomial case. We prove that our bound becomes tight as the marginal contribution of additional features decreases. Both binary and multinomial sparse models are solvable in time almost linear in problem size, representing a very small extra relative cost compared to the classical naive Bayes. Numerical experiments on text data show that the naive Bayes feature selection method is as statistically effective as state-of-the-art feature selection methods such as recursive feature elimination, l1-penalized logistic regression and LASSO, while being orders of magnitude faster. For a large data set, having more than with 1.6 million training points and about 12 million features, and with a non-optimized CPU implementation, our sparse naive Bayes model can be trained in less than 15 seconds.

7.3. Regularity as Regularization: Smooth and Strongly Convex Brenier Potentials in Optimal Transport.

The problem of estimating Wasserstein distances in high-dimensional spaces suffers from the curse of dimensionality: Indeed, ones needs an exponential (w.r.t. dimension) number of samples for the distance between the two samples to be comparable to that between the two measures. Therefore, regularizing the optimal transport (OT) problem is crucial when using Wasserstein distances in machine learning. One of the greatest achievements of the OT literature in recent years lies in regularity theory: one can prove under suitable hypothesis that the OT map between two measures is Lipschitz, or, equivalently when studying 2-Wasserstein distances, that the Brenier convex potential (whose gradient yields an optimal map) is a smooth function. We propose in this work to go backwards, to adopt instead regularity as a regularization tool. We propose algorithms working on discrete measures that can recover nearly optimal transport maps that have small distortion, or, equivalently, nearly optimal Brenier potential that are strongly convex and smooth. For univariate measures, we show that computing these potentials is equivalent to solving an isotonic regression problem under Lipschitz and strong monotonicity constraints. For multivariate measures the problem boils down to a non-convex QCQP problem. We show that this QCQP can be lifted a semidefinite program. Most importantly, these potentials and their gradient can be evaluated on the measures themselves, but can more generally be evaluated on any new point by solving each time a QP. Building on these two formulations we propose practical algorithms to estimate and evaluate transport maps, and illustrate their performance statistically as well as visually on a color transfer task.

7.4. Ranking and synchronization from pairwise measurements via SVD.

Given a measurement graph $G = (V, E)$ and an unknown signal $r \in R^n$, we investigate algorithms for recovering r from pairwise measurements of the form $r_i - r_j; i, j$ in E. This problem arises in a variety of applications, such as ranking teams in sports data and time synchronization of distributed networks. Framed in the context of ranking, the task is to recover the ranking of n teams (induced by r) given a small subset of noisy pairwise rank offsets. We propose a simple SVD-based algorithmic pipeline for both the problem of time synchronization and ranking. We provide a detailed theoretical analysis in terms of robustness against both sampling sparsity and noise perturbations with outliers, using results from matrix perturbation and random matrix theory. Our theoretical findings are complemented by a detailed set of numerical experiments on both synthetic and real data, showcasing the competitiveness of our proposed algorithms with other state-of-the-art methods.

7.5. Polyak Steps for Adaptive Fast Gradient Methods.

Accelerated algorithms for minimizing smooth strongly convex functions usually require knowledge of the strong convexity parameter mu. In the case of an unknown mu, current adaptive techniques are based on restart schemes. When the optimal value f^* is known, these strategies recover the accelerated linear convergence bound without additional grid search. In this paper we propose a new approach that has the same bound without any restart, using an online estimation of strong convexity parameter. We show the robustness of the Fast Gradient Method when using a sequence of upper bounds on mu. We also present a good candidate for this estimate sequence and detail consistent empirical results.

7.6. An Accelerated Decentralized Stochastic Proximal Algorithm for Finite Sums.

Modern large-scale finite-sum optimization relies on two key aspects: distribution and stochastic updates. For smooth and strongly convex problems, existing decentralized algorithms are slower than modern accelerated variance-reduced stochastic algorithms when run on a single machine, and are therefore not efficient. Centralized algorithms are fast, but their scaling is limited by global aggregation steps that result in communication bottlenecks. In this work, we propose an efficient Accelerated Decentralized stochastic algorithm for Finite Sums named ADFS, which uses local stochastic proximal updates and randomized pairwise communications between nodes. On n machines, ADFS learns from nm samples in the same time it takes optimal algorithms to learn from m samples on one machine. This scaling holds until a critical network size is reached, which depends on communication delays, on the number of samples m, and on the network topology. We provide a theoretical analysis based on a novel augmented graph approach combined with a precise evaluation of synchronization times and an extension of the accelerated proximal coordinate gradient algorithm to arbitrary sampling. We illustrate the improvement of ADFS over state-of-the-art decentralized approaches with experiments.

7.7. On Lazy Training in Differentiable Programming.

In a series of recent theoretical works, it was shown that strongly overparameterized neural networks trained with gradient-based methods could converge exponentially fast to zero training loss, with their parameters hardly varying. In this work, we show that this “lazy training” phenomenon is not specific to overparameterized neural networks, and is due to a choice of scaling, often implicit, that makes the model behave as its linearization around the initialization, thus yielding a model equivalent to learning with positive-definite kernels. Through a theoretical analysis, we exhibit various situations where this phenomenon arises in non-convex optimization and we provide bounds on the distance between the lazy and linearized optimization paths. Our numerical experiments bring a critical note, as we observe that the performance of commonly used non-linear deep convolutional neural networks in computer vision degrades when trained in the lazy regime. This makes it unlikely that “lazy training” is behind the many successes of neural networks in difficult high dimensional tasks.

7.8. Implicit Regularization of Discrete Gradient Dynamics in Linear Neural Networks.

When optimizing over-parameterized models, such as deep neural networks, a large set of parameters can achieve zero training error. In such cases, the choice of the optimization algorithm and its respective hyper-parameters introduces biases that will lead to convergence to specific minimizers of the objective. Consequently, this choice can be considered as an implicit regularization for the training of over-parametrized models. In this work, we push this idea further by studying the discrete gradient dynamics of the training of a two-layer linear network with the least-squares loss. Using a time rescaling, we show that, with a vanishing initialization and a small enough step size, this dynamics sequentially learns the solutions of a reduced-rank regression with a gradually increasing rank.

7.9. Efficient Primal-Dual Algorithms for Large-Scale Multiclass Classification.

We develop efficient algorithms to train ℓ_1-regularized linear classifiers with large dimensionality d of the feature space, number of classes k, and sample size n. Our focus is on a special class of losses that includes, in particular, the multiclass hinge and logistic losses. Our approach combines several ideas: (i) passing to the equivalent saddle-point problem with a quasi-bilinear objective; (ii) applying stochastic mirror descent with a proper choice of geometry which guarantees a favorable accuracy bound; (iii) devising non-uniform sampling schemes to approximate the matrix products. In particular, for the multiclass hinge loss we propose a sublinear algorithm with iterations performed in $O(d+n+k)$ arithmetic operations.

7.10. Fast and Faster Convergence of SGD for Over-Parameterized Models (and an Accelerated Perceptron).

Modern machine learning focuses on highly expressive models that are able to fit or interpolate the data completely, resulting in zero training loss. For such models, we show that the stochastic gradients of common loss functions satisfy a strong growth condition. Under this condition, we prove that constant step-size stochastic gradient descent (SGD) with Nesterov acceleration matches the convergence rate of the deterministic accelerated method for both convex and strongly-convex functions. We also show that this condition implies that SGD can find a first-order stationary point as efficiently as full gradient descent in non-convex settings. Under interpolation, we further show that all smooth loss functions with a finite-sum structure satisfy a weaker growth condition. Given this weaker condition, we prove that SGD with a constant step-size attains the deterministic convergence rate in both the strongly-convex and convex settings. Under additional assumptions, the above results enable us to prove an $O(1/k^2)$ mistake bound for k iterations of a stochastic perceptron algorithm using the squared-hinge loss. Finally, we validate our theoretical findings with experiments on synthetic and real datasets.

7.11. Globally Convergent Newton Methods for Ill-conditioned Generalized Self-concordant Losses.

In this project, we study large-scale convex optimization algorithms based on the Newton method applied to regularized generalized self-concordant losses, which include logistic regression and softmax regression. We first prove that our new simple scheme based on a sequence of problems with decreasing regularization parameters is provably globally convergent, that this convergence is linear with a constant factor which scales only logarithmically with the condition number. In the parametric setting, we obtain an algorithm with the same scaling than regular first-order methods but with an improved behavior, in particular in ill-conditioned problems. Second, in the non parametric machine learning setting, we provide an explicit algorithm combining the previous scheme with Nyström projection techniques, and prove that it achieves optimal generalization bounds with a time complexity of order $O(nd_{eff}(\lambda))$, a memory complexity of order $O(d_{eff}(\lambda)^2)$ and no dependence on the condition number, generalizing the results known for least-squares regression. Here n is the number of observations and df λ is the associated degrees of freedom. In particular, this is the first large-scale algorithm to solve logistic and softmax regressions in the non-parametric setting with large condition numbers and theoretical guarantees.

7.12. Efficient online learning with kernels for adversarial large scale problems

We are interested in a framework of online learning with kernels for low-dimensional but large-scale and potentially adversarial datasets. We study the computational and theoretical performance of online variations of kernel Ridge regression. Despite its simplicity, the algorithm we study is the first to achieve the optimal regret for a wide range of kernels with a per-round complexity of order n^{α} with $\alpha < 2$. The algorithm we consider is based on approximating the kernel with the linear span of basis functions. Our contributions is two-fold: 1) For the Gaussian kernel, we propose to build the basis beforehand (independently of the data) through Taylor expansion. For d-dimensional inputs, we provide a (close to) optimal regret of order $O((logn)^{d+1})$ with per-round time complexity and space complexity $O((logn)^{2d})$. This makes the algorithm a suitable choice as soon as $n \geq e^{d}$ which is likely to happen in a scenario with small dimensional and large-scale dataset; 2) For general kernels with low effective dimension, the basis functions are updated sequentially in a data-adaptive fashion by sampling Nyström points. In this case, our algorithm improves the computational trade-off known for online kernel regression

7.13. Affine Invariant Covariance Estimation for Heavy-Tailed Distributions

In this work we provide an estimator for the covariance matrix of a heavy-tailed multivariate distribution. We prove that the proposed estimator $\widehat{S}$ admits an *affine-invariant* bound of the form

$$(1-\epsilon)S \leq \widehat{S}(1+\epsilon)S$$

in high probability, where S is the unknown covariance matrix, and $\leq$ is the positive semidefinite order on symmetric matrices. The result only requires the existence of fourth-order moments, and allows for $\epsilon = O(\sqrt{k^4 dlog(d/\delta)/n})$ where k^4 is a measure of kurtosis of the distribution, d is the dimensionality of the space, n is the sample size, and $1-\delta$ is the desired confidence level. More generally, we can allow for regularization with level λ, then d gets replaced with the degrees of freedom number. Denoting $cond(S)$ the condition number of S, the computational cost of the novel estimator is $O(d^2 n + d^3 log(cond(S)))$, which is comparable to the cost of the sample covariance estimator in the statistically interesting regime $n \geq d$. We consider applications of our estimator to eigenvalue estimation with relative error, and to ridge regression with heavy-tailed random design.

7.14. Beyond Least-Squares: Fast Rates for Regularized Empirical Risk Minimization through Self-Concordance

We consider learning methods based on the regularization of a convex empirical risk by a squared Hilbertian norm, a setting that includes linear predictors and non-linear predictors through positive-definite kernels. In order to go beyond the generic analysis leading to convergence rates of the excess risk as $O(\sqrt{1/n})$ from n observations, we assume that the individual losses are self-concordant, that is, their third-order derivatives are bounded by their second-order derivatives. This setting includes least-squares, as well as all generalized linear models such as logistic and softmax regression. For this class of losses, we provide a bias-variance decomposition and show that the assumptions commonly made in least-squares regression, such as the source and capacity conditions, can be adapted to obtain fast non-asymptotic rates of convergence by improving the bias terms, the variance terms or both.

7.15. Statistical Estimation of the Poincaré constant and Application to Sampling Multimodal Distributions

Poincaré inequalities are ubiquitous in probability and analysis and have various applications in statistics (concentration of measure, rate of convergence of Markov chains). The Poincaré constant, for which the inequality is tight, is related to the typical convergence rate of diffusions to their equilibrium measure. In this paper, we show both theoretically and experimentally that, given sufficiently many samples of a measure, we can estimate its Poincaré constant. As a by-product of the estimation of the Poincaré constant, we derive an algorithm that captures a low dimensional representation of the data by finding directions which are difficult to sample. These directions are of crucial importance for sampling or in fields like molecular dynamics, where they are called reaction coordinates. Their knowledge can leverage, with a simple conditioning step, computational bottlenecks by using importance sampling techniques.

7.16. Stochastic first-order methods: non-asymptotic and computer-aided analyses via potential functions

We provide a novel computer-assisted technique for systematically analyzing first-order methods for optimization. In contrast with previous works, the approach is particularly suited for handling sublinear convergence rates and stochastic oracles. The technique relies on semidefinite programming and potential functions. It allows simultaneously obtaining worst-case guarantees on the behavior of those algorithms, and assisting in choosing appropriate parameters for tuning their worst-case performances. The technique also benefits from comfortable tightness guarantees, meaning that unsatisfactory results can be improved only by changing the setting. We use the approach for analyzing deterministic and stochastic first-order methods under different assumptions on the nature of the stochastic noise. Among others, we treat unstructured noise with bounded variance, different noise models arising in over-parametrized expectation minimization problems, and randomized block-coordinate descent schemes.

7.17. Optimal Complexity and Certification of Bregman First-Order Methods

We provide a lower bound showing that the O(1/k) convergence rate of the NoLips method (a.k.a. Bregman Gradient) is optimal for the class of functions satisfying the h-smoothness assumption. This assumption, also known as relative smoothness, appeared in the recent developments around the Bregman Gradient method, where acceleration remained an open issue. On the way, we show how to constructively obtain the corresponding worst-case functions by extending the computer-assisted performance estimation framework of Drori and Teboulle (Mathematical Programming, 2014) to Bregman first-order methods, and to handle the classes of differentiable and strictly convex functions.

7.18. Efficient First-order Methods for Convex Minimization: a Constructive Approach

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 technique builds upon a certain variant of the conjugate gradient method to construct a family of methods such that a) all methods in the family share the same worst-case guarantee as the base conjugate gradient method, and b) the family includes a fixed-step first-order method. We demonstrate the effectiveness of the approach by deriving optimal methods for the smooth and non-smooth cases, including new methods that forego knowledge of the problem parameters at the cost of a one-dimensional line search per iteration, and a universal method for the union of these classes that requires a three-dimensional search per iteration. In the strongly convex case, we show how numerical tools can be used to perform the construction, and show that the resulting method offers an improved worst-case bound compared to Nesterov's celebrated fast gradient method.

TAU Project-Team

7. New Results

7.1. Toward Good AI

7.1.1. Causal Modeling

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag;
PhDs: Diviyan Kalainathan
Collaboration: David Lopez-Paz (Facebook).

The search for **causal models** relies on quite a few hardly testable assumptions, e.g. causal sufficiency [160]; 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 [112] 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 [114]. An edited book has been published [48], that somewhat summarizes the whole history of Cause-EFfect Paris research. Several chapters of this book have co-authors in TAU: *Evaluation methods of cause-effect pairs* [49], *Learning Bivariate Functional Causal Models* [47], *Discriminant Learning Machines* [51], and *Results of the Cause-Effect Pair Challenge* [50].

In D. Kalainathan's PhD [14] and O. Goudet's postdoc, the search for causal models has been tackled in the framework of generative networks [107], 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. CGNN favorably compares with the state of the art w.r.t. usual performance indicators (AUPR, SID) on main causal benchmarks, though with a large computational cost.

An attempt to scale up causal discovery, we proposed the Structural Agnostic Model approach [14] [120]. Working directly on the observational data, this global approach implements a variant of the popular adversarial game [99] 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 input variables, yielding a sparse causal graph. SAM obtains state-of-the-art performances on causal benchmarks, and scales up to a few hundred variables.

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
PhD: Marc Nabhan

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 [143] 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 of first impressions analysis [57].

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, to provide understandable explanations on its results. Kickoff took place in September 2019, and we are still looking for good post-doc candidates.

Note also that the on-going work on the identification of the border of the failure zone in the parameter space of the autonomous vehicle simulator [37] (Section 7.1.3) also pertains to explainability.

Finally, a completely original approach to DNN explainability might arise from the study of structural glasses (7.2.3), with a parallel to Graph Neural Networks (GNNs), that could become an excellent non-trivial example for developing explainability protocols.

7.1.3. Robustness of AI Systems

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhDs: Julien Girard, Marc Nabhan, Nizham Makhoud
Collaboration: Zakarian Chihani (CEA); Hiba Hage and Yves Tourbier (Renault); Johanne Cohen (LRI-GALAC) and Christophe Labreuche (Thalès)

As said (Section 3.1.2 , TAU is considering two directions of research related to the certification of MLs. The first direction, related to formal approaches, is the topic of Julien Girard's PhD (see also Section 3.1.2). On the opposite, the second axis aims to increase the robustness of systems that can only be experimentally validated. Two paths are investigated in the team: assessing the coverage of the datasets (more particularly here, used to train an autonomous vehicle controller), topic of Marc Nabhan's CIFRE with Renault; and detecting flaws in the system by reinforcement learning, as done by Nizam Makdoud's CIFRE PhD with Thalès THERESIS.
Formal validation of Neural Networks
The topic of provable deep neural network robustness has raised considerable interest in recent years. Most research in the literature has focused on adversarial robustness, which studies the robustness of perceptive models in the neighbourhood of particular samples. However, other works have proved global properties of smaller neural networks. Yet, formally verifying perception remains uncharted. This is due notably to the lack of relevant properties to verify, as the distribution of possible inputs cannot be formally specified. With Julien Girard-Satabin's PhD thesis, we propose to take advantage of the simulators often used either to train machine learning models or to check them with statistical tests, a growing trend in industry. Our formulation [34] allows us to formally express and verify safety properties on perception units, covering all cases that could ever be generated by the simulator, to the difference of statistical tests which cover only seen examples. Along with this theoretical formulation, we provide a tool to translate deep learning models into standard logical formulae. As a proof of concept, we train a toy example mimicking an autonomous car perceptive unit, and we formally verify that it will never fail to capture the relevant information in the provided inputs.
Experimental validation of Autonomous Vehicle Command 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 step ii) within Marc Nabhan's CIFRE PhD (defense expected in Sept. 2020). The current target scenario is the insertion of a car on a motorway, the "drosophila" of autonomous car scenarios and the goal is 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, and the identification of the borders of the failure zone using an as simple as possible description, thus allowing engineers to understand the reasons for the flaws. A first paper was published [37] proposing several approaches for the identification of failures. On-going work is concerned with a precise yet simple definition of the border of the failure zone.

Reinforcement Learning from Advice In the context of his CIFRE PhD with Thalès, Nizam Makdoud tests (in simulation) physical security systems using reinforcement learning to learn the best sequence of action that will break through the system. This lead him to propose an original approach called *LEarning from Advice* (LEA) that uses knowledge from several policies learned on different tasks. Whereas Learning by imitation uses the actions of the known policy, the proposed method uses the different Q-functions of the known policies. The main advantage of this strategy is its robustness to poor advice, as the policy then reverts to standard DDPG [127]. The results (submitted) demonstrate that LEA is able to learn faster than DDPG if given good-enough policies, and only slightly slower when given lousy advices.

Learning Multi-Criteria Decision Aids (Hierarchical Choquet models) In collaboration with Johanne Cohen (LRI-GALAC) and Christophe Labreuche (Thalès), the representation and data-driven elicitation of hierarchical Choquet models has been tackled. A specific neural architecture, enforcing by design the model constraints (monotonicity, additivity), and supporting the end-to-end training of the Multi-Criteria Decision aid, has been proposed in Roman Bresson's PhD. Under mild assumptions, an identifiability result (existence and unicity of the sought model in the neural space) is obtained. The approach is empirically validated and successfully compared to the state of the art.

7.2. Learning to Learn

*7.2.1. Auto-**

Participants: Guillaume Charpiat, Isabelle Guyon, Marc Schoenauer, Michèle Sebag

PhDs: Léonard Blier, Guillaume Doquet, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun, Pierre Wolinski

Collaboration: Vincent Renault (SME Artelys); Yann Ollivier (Facebook)

Auto-☆ studies at TAU investigate several research directions.

As mentioned in Section 3.3 , a popular approach for algorithm selection is collaborative filtering. In Lisheng Sun's PhD [15], active learning was used on top of the CofiRank algorithm for matrix factorization [164], improving the results and the time to solution of the recommendation algorithm. Furthermore, 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. Another contribution in Lisheng's PhD is an extension of AutoSklearn that detects concept drifts and corrects the current model accordingly.

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 MOSAIC algorithm performs on par with AutoSklearn, the winner of Auto-☆ international competitions in the last few years.

Auto-☆ would be much easier if appropriate and affordable meta-features (describing datasets) were available. Taking inspiration from equivariant learning [144] and learning from distributions [130], on-going work aims to learn such meta-features, based on the OpenML archive [161].

A key building block in Auto-☆ lies in the data preparation and specifically variable selection. Guillaume Doquet's PhD [13] addresses the problem of agnostic feature selection, independently of any target variable. The point d'orgue of his work is Agnos [32] (Best Paper Award at ECML 2019), that combines an AutoEncoder with structural regularizations to sidestep the combinatorial optimization problem at the core of feature selection. The extensive experimental validation of AgnoS on the scikit-feature benchmark suite demonstrates its ability compared to the state of the art, both in terms of supervised learning and data compression.
Several works have focused on the adjustment of specific hyper-parameters for neural nets. Pierre Wolinski's PhD (to be defended in January 2020, publication submitted) studies three such hyper-parameters: i) network width (number of neurons in each layer); ii) regularizer importance in the objective function to minimize (factor balancing data term and regularizer); and iii) learning rate. Regarding the network width, it is adjusted during training thanks to a criterion quantifying each neuron's importance, naturally leading to a sparsification effect (as for L1 norm minimization). This study is actually extendable to not only layers' widths but also layers' connectivity (e.g., in modern networks where each layer may be connected to any other layer with 'skip' connections). Regarding the regularizer weight, it is formulated as a probabilistic prior from a Bayesian perspective, which leads to a particular value that the regularizer weight should have in order the network to satisfy some property. Regarding the learning rate, Pierre Wolinski and Leonard Blier [27] proposed to attach fixed learning rates to each neuron (picked randomly) and calibrate this learning rate distribution in such a way that neurons are sequentially active, learning in an optimally agile manner during a first learning phase, and being stable in later phases. This remove the need to tune the learning rate.
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 [154], and steadily contributes to the organization of new challenges (Section 7.6).

7.2.2. Deep Learning: Practical and 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), Y. Tarabalka (Inria Titane)

Although a comprehensive mathematical theory of deep learning is yet to come, theoretical insights from information theory or from dynamical systems can deliver principled improvements to deep learning and/or explain the empirical successes of some architectures compared to others.

In his PhD [16], Corentin Tallec presents several contributions along these lines:

- In [158], it is shown that the LSTM structure can be understood from axiomatic principles, enforcing the *robustness of the learned model to temporal deformation (warpings) in the data*. The complex LSTM architecture, introduced in the 90's, has become the currently dominant architecture for modeling temporal sequences (such as text) in deep learning. It is shown that this complex LSTM architecture necessarily arises if one wants the model to be able to handle time warpings in the data (such as arbitrary accelerations or decelerations in the signal), and their complex equations can be derived axiomatically.
- In [132] (oral presentation at ICML 2018) the issue of mode dropping in adversarial generative models is tackled using information theory. The adversary (discriminator) task is set to predict the proportion of true and fake images in a set of images, via an information theory criterion, thus working at the level of the *overall distribution* of images. The discriminator is thus mande more able to detect statistical imbalances between the modes created by the generator, thereby reducing the mode dopping phenomenon. The proposed architecture, inspired from equivariant approaches, is provably able to detect all permutation-invariant statistics in a set of images.
- In [159], the problem of recurrent network training is tackled via the theory of dynamical systems by proposing a simple fully online solution avoiding the "time rewind" step, based on real-time, noisy but unbiased approximations of model gradients, which can be implemented easily in a black-box fashion on top of any recurrent model, and which is well-justified mathematically. The price to pay is an increase of variance.

- In [42], we identify sensitivity to time discretization of Deep RL in near continuous-time environments as a critical factor. Empirically, we find that Q-learning-based approaches collapse with small time steps. Formally, we prove that Q-learning does not exist in continuous time. We detail a principled way to build an off-policy RL algorithm that yields similar performances over a wide range of time discretizations, and confirm this robustness empirically.

Several other directions have been investigated: In [41], 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.

Another direction regards the topology induced by a trained neural net, and how similar are two samples in the NN perspective. The definition proposed in [29] relies on varying the NN parameters and examining whether the impacts of this variation on both samples are aligned. The mathematical properties of this similarity measure are investigated and the similarity is shown to define a kernel on the input space. This kernel can be used to tractably estimate the sample density, and it leads to new directions for the statistical learning analysis of NN, e.g. in terms of additional loss (requiring that similar examples have a similar latent representation in the above sense) or in terms of resistance to noise. Specifically, a multimodal image registration task is presented where almost perfect accuracy is reached, despite a high label noise (see Section 7.5.2). Such an impressive self-denoising phenomenon can be explained and quantified as a noise averaging effect over the labels of similar examples.

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).; Clément Vignax (EPFL); Yufei Han (Symantec).

The information content of a trained restricted Boltzmann machine (RBM) can be analyzed by comparing the singular values/vectors of its weight matrix, referred to as modes, to that of a random RBM (typically following a Marchenko-Pastur distribution) [83]. The analysis of a single learning trajectory is replaced by analyzing the distribution of a well chosen 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 [84]. Although simplifying assumptions are required for a mean-field analysis in closed form of the above distribution, it nevertheless delivers some simple heuristics to speed up the learning convergence and to simplify the models.

This analysis will be extended along two directions: handling missing data [58]; and considering exactly solvable RBM (non-linear RBM for which the contrastive divergence can be computed in closed forms, e.g. using a spherical model) [54]. W.r.t. missing data, state of the art results have been obtained on semi-supervised tasks in the context of Internet-of-Things security, considering a high rate of missing inputs and labels). On the theoretical side exact generic RBM learning trajectories have been characterized, showing intriguing connections based on Bose-Einstein condensation mechanism associated to information storing. Our collaboration with J. Rocchi(LPTMS, Univ. Paris Sud) aims to characterize the landscape of RBMs learned from different initial conditions, and to relate this landscape to the number of parameters (hidden nodes) of the system.

An emerging research topic, concerns the interpretation of deep learning by means of Gaussian processes and associated neural tangent limit kernel in the thermodynamical limit obtained by letting layer's width go to infinity [118]. Various things are planned to be investigated on the basis of this theoretical tool in particular how this translate to RBM or DBM setting, and whether a double dip behaviour is to be expected as well for generative models.

As mentioned earlier, the use of ML to address fundamental physics problems is quickly growing. This leads to some methodological mistakes from newcomers, that have been investigated by Rémi Perrier (2 month internship). 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 can then help identifying "computational order parameters", that would advance the understanding of physical phenomena [19], on the one hand, and support the development of more complex models, on the other hand. More generally, attacking the problem of amorphous condensed matter by novel Graph Neural Networks (GNN) architectures is a very promising lead, regardless of the precise quantity one may want to predict. Currently GNNs are engineered to deal with molecular systems and/or crystals, but not to deal with amorphous matter. This second axis is currently being attacked in collaboration with Clément Vignac (PhD Student at EPFL), using GNNs. Furthermore, this problem is new to the ML community and it provides 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. While the simultaneous advent of massive data and unprecedented computational power has opened exciting new avenues, it has also raised new questions and challenges.

Several studies are being conducted in TAU, about labor (labor markets, platform "micro-work", 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
PhDs: Diviyan Kalainathan, Guillaume Bied, Armand Lacombe
Post-Docs: Saumya Jetley
Engineers: Raphael Jaiswal, Victor Alfonso Naya
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Antonio Casilli, Ulrich Laitenberger (Telecom Paris); Odile Chagny (IRES); Alessandro Delfanti (University of Toronto)

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 Two projects deal with the domain of job markets and machine learning. The DATAIA project Vadore, in collaboration with ENSAE and Pôle Emploi, has two goals. First, to improve the recommendation of jobs for applicants (and the recommendation of applicants to job offers). The main originalities in this project are: i) to use both machine learning and optimal transport to improve the recommendation by learning a matching function for past hiring, and then to apply optimal transport-like bias to tackle market congestion (e.g. to avoid assigning many applicants to a same job offer); ii) to use randomized test on micro-markets (AB testing) in collaboration with Pôle Emploi to test the global impact of the algorithms.

The JobAgile project, BPI-PIA contract, coll. EHESS, Dataiku and Qapa, deals with low salary interim job recommendations. A main difference with the Vadore project relies on the high reactivity of the Qapa and Dataiku startups: i) to actually implement AB-testing; ii) to explore related functionalities, typically the recommendation of formations; iii) to propose a visual querying of the job market, using the Cartolabe framework (below).

The platform economy and digital labor

Another topic concerns the digital economy and the transformations of labor that accompany it. One part of the platform economy carries promises of social, not only techno-economic, innovation. If enthusiasms for a new "sharing economy" or "collaborative economy" have progressively faded away, values of decentralization, autonomy, and flatter coordination are still commonly associated to platforms. A conference paper by P. Tubaro studies how events constitute places where actors of the platform economy negotiate values and collectively drive forms of social change [43].

The platform economy and its effects on labor are also linked to the current developments of AI [22]. In collaboration with A.A. Casilli (Telecom ParisTech), P. Tubaro has received funding from the Union Force Ouvrière, from France Stratégie (a Prime Minister's service), and from MSH Paris-Saclay, to map "micro-work" in France (DiPLab project). The term micro-work refers to small, data-related tasks that are performed online against low remunerations, such as tagging objects in images, transcribing bits of text, and recording utterances aloud. Specialized platforms such as Amazon Mechanical Turk, Clickworker and Microworkers recruit online providers to execute these tasks for their clients, mostly for data-intensive production processes. In addition to poor working conditions and low pay, micro-work raises issues in terms of privacy and data protection, insofar as outside providers are entrusted with data that may include personal information [23].

The results of the DiPLab study were published in a report that attracted significant media attention [52], and presented as part of a large event on micro-work at the headquarters of France Stratégie in June 2019. Two articles relying on DiPlab results, one of which was first published as a working paper [62], [61], are now under review.

A joint franco-Canadian grant obtained by P. Tubaro and A. Delfanti (University of Toronto) enabled the creation of an "International Network on Digital Labor", aiming to bring together scholars interested in various forms of digital platform labor. Inauguration of the network involved the organization of two workshops, one in Paris (June 2019) and the other in Toronto (October 2019).

Further research on how digital platforms transform labor practices and affect the very definition of professions is being undertaken by P. Tubaro as part of a two-year (2018-2020) grant from DARES (French Ministry of Labor), in collaboration with O. Chagny of IRES, a union-funded think-tank), and A.A. Casilli (Telecom ParisTech).

A newly-obtained grant from ANR (with A.A. Casilli and U. Laitenberger, Telecom ParisTech) will enable P. Tubaro to further explore the global production networks that link AI developers and producers to data-related work across national boundaries, following outsourcing chains that extend from France to French-speaking African countries, and from Spain and the USA to parts of Latin America. This new project, entitled "The HUman Supply cHain behind smart technologies" (HUSH), will start in January 2020.

7.3.2. Health, food, and socio-demographic relationships

Participants: Philippe Caillou, Michèle Sebag, Paola Tubaro
Post-doc: Ksenia Gasnikova
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> One project motivation is the fact that general recommendations (e.g., *Eat 5 fruit and vegetable per day*) are hardly effective on populations at risk. 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 of obesity, or a consequence thereof, or both a cause and a consequence. A main difficulty is the lack of control populations to assess a diet impact. Such a control population could be approximated in the case of the organic diet, showing a statistically significant impact of this diet on the BMI distribution. The question of finding confounders (e.g. based on wealth or education) or "backdoor" variables in under study.

7.3.3. Scientific Information System and Visual Querying

Participants: Philippe Caillou, Michèle Sebag
Engineers: Anne-Catherine Letournel, Jonas Renault
Collaboration: Jean-Daniel Fekete (AVIZ, Inria Saclay)

A third area of activity concerns the 2D visualisation and querying of a corpus of documents. Its initial motivation was related to scientific organisms, institutes or Universities, using their scientific production (set of articles, authors, title, abstract) as corpus. 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 extensions, as an open-source platform, are under submission at the time of writing.

The originality of the approach is to rely on the content of the documents (as opposed to, e.g. the graph of co-authoring and citations). This specificity allowed to extend Cartolabe to various corpora, such as Wikipedia, Bibliotheque Nationale de France, or the Software Heritage. Cartolabe was also applied in 2019 to the *Grand Debat* dataset: to support the interactive exploration of the 3 million propositions; and to check the consistency of the official results of the *Grand Debat* with the data.

Among its intended functionalities are: the visual assessment of a domain and its structuration (who is expert in a scientific domain, how related are the domains); the coverage of an institute expertise relatively to the general expertise; the evolution of domains along time (identification of rising topics). A round of interviews with beta-user scientists is under way since end 2019. Cartolabe usage raises questions at the crossroad of human-centered computing, data visualization and machine learning: i) how to deal with stressed items (the 2D projection of the item similarities poorly reflects their similarities in the high dimensional document space; ii) how to customize the similarity and exploit the users' feedback about relevant neighborhoods.

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 focus of the development team in 2019 was on the stability of the platform and on the documentation to provide a stable and well documented framework to the users.

7.4. Energy Management

7.4.1. Power Grids Daily Management

Participants: Isabelle Guyon, Marc Schoenauer

PhDs: Benjamin Donnot, Balthazar Donon
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Olivier Teytaud (Facebook)

Benjamin Donnot's CIFRE PhD with RTE [12] dealt with Power Grid safety: The goal is to assess in real time the so-called "(n-1) safety" (see Section 4.2) of possible recovery actions modifying the topology of the grid after some problem occurred somewhere on the grid. However, the HADES 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 of a tentative topology. A simplified simulator is also available, but its accuracy is too poor to give good results. Deep surrogate models can be trained off-line for a given topology, based on the results of the slow simulator, with high-enough 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. Nevertheless, this approach poorly generalize to topologies outside the distribution of the ones used for training.

An original "guided dropout" approach was first proposed [87], in which the topology directly acts on the connections of the deep network: a missing line suppresses some connections. 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 experimentally validated against the one-hot encoding on small subsets of the French grid (up to 308 lines). Interestingly, and rather surprisingly, 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 [86] 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.

The guided dropout approach has been further extended and generalized with the LEAP (Latent Encoding of Atypical Perturbation) architecture [30], [17], by crossing-out connections between the encoder and the decoder parts of the ResNet architecture. LEAP then performs transfer learning over spaces of distributions of topology perturbations, allowing to better handle more complex actions on the tolology, going beyond (n-1) and (n-2) perturbations by also including node-split, a current action in the real world. The LEAP approach was theoretically studied in the case of additive perturbations, and experimentally validated on an actual sub-grid of the French grid with 46 consumption nodes, 122 production nodes, 387lines and 192 substations.

LEAP is also the firs part of Balthazar Donon's on-going PhD, that currently develops using a completely different approach to approximate the power flows on a grid, i.e. that of Graph Neural Networks (GNNs). From a Power Grid perspective, GNNs can be viewed as including the topology in the very structure of the neural network, and learning some generic transfer function amongst nodes that will perform well on any topology. First results [31] use a loss based on a large dataset of actual power flows computed using the slow HADES simulator. The results indeed generalize to very different topologies than the ones used for training, in particular very different sizes of power grids. On-going work [56] removes the need to run HADES thanks to a loss that directly aims to minimize Kirshoff's law on all lines.

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.

Regarding the design of such grids, and provided accurate predictions of consumption are available (see below), off-the-shelf graph optimization algorithms can be used. Berna Batu is gathering different approaches. Herilalaina Rakotoarison's PhD tackles the automatic tuning of their parameters (see Section 7.2.1); while the Mosaic algorithm is validated on standard AutoML benchmarks [40], its application to Artelys' home optimizer at large Knitro is on-going, 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. The concept of *Compositional Variational Auto-Encoder* was proposed: it is amenable to multi-ensemblist operations (addition or subtraction of elements in the composition), enabled by the invariance and generality of the whole framework w.r.t. respectively, the order and number of the elements. It has been first tested on synthetic problems [26].

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 [93] 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 [68] and the TRrackML challenge [46]. 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 (AD) is the subject of A. Pol's 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. [21] 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. The result has been included in the production suite of the CMS experiment at CERN. Recent work has focused on improving AD for the trigger system, which is the first stage of event selection process in most experiments at the LHC at CERN. The hierarchical structure of the trigger process called for exploiting the advances in modeling complex structured representations that perform probabilistic inference effectively, and specifically variational autoencoders. Previous works argued that training VAE models only with inliers is insufficient and the framework should be significantly modified in order to discriminate the anomalous instances. In this work, we exploit the deep conditional variational autoencoder (CVAE) and we define an original loss function together with a metric that targets hierarchically structured data AD [39], [64]. This results in an effective, yet easily trainable and maintainable model.

The highly visible TrackML challenge [46] 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 $\times$ 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).

These last years, 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 [133] and, soon after, larger ones by GAFAM).

This year, we continued the work started in [167] about the registration of remote sensing images (RGB pictures) with cadastral maps (made of polygons indicating buildings and roads). We extended it in [33] to the case of real datasets, i.e. to noisy data. Indeed, in remote sensing, datasets are often large but of poor ground truth annotation quality. It turns out that, when training on datasets with noisy labels, one can still obtain accuracy scores far better than the noise variance in the training set, due to averaging effects over the labels of similar examples. To properly explain this, a theoretical study was conducted (cf. Section 7.2.2). Given any already trained neural network and its noisy training set, without knowing the real ground truth, we were then able to quantify this noise averaging effect [29].

We also tackled the problem of pansharpening, i.e. the one of producing a high-resolution color image, given a low-resolution color image and a high-resolution greyscale one [35], with deep convolutional neural networks as well.

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 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). 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*. This project has been articulated around Mandar Chandorkar's Phd thesis[11] which has been defended this year in Eindhoven. One

[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.

of the main result that has been obtained concerns the prediction of solar wind impacting earth magnetosphere from solar images. In this context 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. We have provided in[28] an approach to this problem combining deep learning and an original Bayesian forward attention mechanism. A theoretical analysis based on linear stability has been proposed to put this algorithm on firm ground. From the practical point of view, encouraging tests have been performed both on synthetic data and real data with results slightly better than those present in the specialized literature on a small dataset. Various extension of the method, of the experimental tests and of the theoretical analysis are planned.

7.5.4. Genomic Data and Population Genetics

Participants: Guillaume Charpiat, Flora Jay, Aurélien Decelle, Cyril Furtlehner
PhD: Théophile Sanchez – **PostDoc**: Jean Cury
Collaboration: Bioinfo Team (LRI), Estonian Biocentre (Institute of Genomics, Tartu, Estonia), Pasteur Institute (Paris), TIMC-IMAG (Grenoble)

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.

We developed an approach that extracts features from genomic data using deep neural networks and combines them with a Bayesian framework to approximate the posterior distribution of demographic parameters. The key difficulty is to build flexible problem-dependent architectures, supporting transfer learning and in particular handling data with variable size. 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 and compared their performances to state-of-the-art approaches [148]. In the short-term these architectures can be used for demographic inference or selection inference in bacterial populations (ongoing work with a postdoctoral researcher, J Cury, and the Pasteur Institute); the longer-term goal is to integrate them in various systems handling genetic data or other biological sequence data.

In collaboration with the Institute of Genomics of Tartu (Estonia; B Yelmen, 3-month visitor at LRI), we leveraged two types of generative neural networks (Generative Adversarial Networks and Restricted Boltzmann Machines) to learn the high dimensional distributions of real genomic datasets and create artificial genomes [66]. These artificial genomes retain important characteristics of the real genomes (genetic allele frequencies and linkage, hidden population structure, ...) without copying them and have the potential to be valuable assets in future genetic studies by providing anonymous substitutes for private databases (such as the ones hold by companies or public institutes like the Institute of Genomics of Tartu). Yet, ensuring anonymity is a challenging point and we measured the privacy loss by using and extending the Adversarial Accuracy score developed by the team for synthetic medical data [44].

In collaboration with TIMC-IMAG, we proposed a new factor analysis approach that process genetic data of multiple individuals from present-day and ancient populations to visualize population structure and estimate admixture coefficients (that is, the probability that an individual belongs to different groups given the genetic data). This method corrects the traditionally-used PCA by accounting for time heterogeneity and enables a more accurate dimension reduction of paleogenomic data [59].

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, with the goal of exploring and sampling all possible configuration basins of given molecules. 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. This year, we studied how to bypass simulations by directly predicting, given a molecule formula, its possible configurations. This is done using Graph Neural Networks [89] in a generative way, producing 3D configurations. The goal is to sample all possible configurations, and with the right probability.

7.5.6. Storm trajectory prediction

Participants: Guillaume Charpiat
Collaboration: Sophie Giffard-Roisin (IRD), Claire Monteleoni (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 [169]. 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. The continuation of the work started last year [101] shows that with deep learning one can outperform the state-of-the-art in many cases [18].

7.6. Challenges

Participants: Cécile Germain, Isabelle Guyon, Adrien Pavao, Anne-Catherine Letournel, Michèle Sebag
PhD: Zhengying Liu, Lisheng Sun, Balthazar Donon
Collaborations: D. Rousseau (LAL), André Elisseeff (Google Zurich), Jean-Roch Vilmant (CERN), Antoine Marot and Benjamin Donnot (RTE), Kristin Bennett (RPI), Magali Richard (Université de Grenoble).

The TAUgroup uses challenges (scientific competitions) as a means of stimulating research in machine learning and engage a diverse community of engineers, researchers, and students to learn and contribute advancing the state-of-the-art. The TAUgroup is community lead of the open-source **Codalab** platform, hosted by Université Paris-Saclay. The project had grown in 2019 and includes now an engineer dedicated full time to administering the platform and developing challenges (Adrien Pavao), financed by a new project just starting with the Région Ile-de-France. This project will also receive the support of the Chaire Nationale d'Intelligence Artificielle of Isabelle Guyon for the next four years.

Following the highly successful ChaLearn **AutoML** Challenges (NIPS 2015 – ICML 2016 [111] – PKDD 2018 [113]), a series of challenges on the theme of **AutoDL** [129] was run in 2019 (see http://autodl.chalearn.org, addressing the problem of tuning the hyperparameters of Deep Neural Networks, including the topology of the network itself. Co-sponsored by Google Zurich, it required participants to upload their code on the Codalab platform. The series included two challenges in computer vision called **AutoCV** and **AutoCV2**, to promote automatic machine learning for image and video processing, in collaboration with University of Barcelona [45]. It also included challenges in speech processing (**AutoSpeech**), text processing (**AutoNLP**), weakly supervised learning (**AutoWeakly**) and times series (**AutoSeries**), co-organized with 4Paradigm. It culminated with launching the **AutoDL** challenge combining multiple modalities (presently on-going). The winners of each challenge open-sourced their code. GPU cloud resources were donated by Google. AutoDL was an official NeurIPS 2020 competition.

Part of the High Energy Physics activities of the team, **TrackML** [79], [80] first phase was run and co-sponsored by Kaggle, until September 2018. The second phase has been run on Codalab until March 2019, requiring code submission; algorithms were then ranked by combining accuracy and speed. The best submissions largely outperform the existing solutions. The challenge has been presented at NeurIPS [46], and at a CERN workshop[0]. 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.

A new challenge series in Reinforcement Learning was started with the company RTE France, one the theme “Learning to run a power network” [134] (**L2RPN**, http://l2rpn.chalearn.org). The goal is to test the potential of Reinforcement Learning to solve a real world problem of great practical importance: controlling electricity transportation in smart grids while keeping people and equipment safe. The first edition was run in Spring 2019 and was part of the official selection of the IJCNN 2019 conference. It ran on the Codalab platform coupled with the open source PyPower simulator of power grids interfaced with the Opengym RL framework, developed by OpenAI. In this gamified environment, the participants had to create a proper controller of a small grid of 14 nodes. Not all of them used RL, but some combinations of RL and human expertise proved to be competitive. In 2020, we will launch a new edition of the challenge with a more powerful simulator rendering the grid more realistic and capable of simulating a 118-node grid within our computational constraints. This competition was already accepted as part of the official program of IJCNN 2020.

The **HADACA** project (EIT Health) aims to run a series of challenges to promote and encourage innovations in data analysis and personalized medicine. Université de Grenoble organized a challenge on matrix factorization (https://www.medinfo-lyon.org/en/matrixen) using Codalab. The challenge gathered transdisciplinary instructors (researchers and professors), students, and health professionals (clinicians). The HADACA project contributed to create a large dataset to assess tumor heterogeneity in cancer research as well as developing innovative pedagogical methods to sensitize students to big data analysis in health. One of the products of HADACA is the ChaGrade platform (https://chagrade.lri.fr/), a tool allowing instructors to easily use challenges in the classroom, grading them as homework, and monitoring submissions and progress. HADACA will be pursued in 2020 by a sequel project also funded by EIT Health, called COMETH. The objective of COMETH will be to create an environment to conduct systematic benchmarks, based on Codalab. 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.

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 [38] : 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. Codalab has also been used to implement reinforcement learning homework in the form of challenges by Victor Berger and Heri Rakotoarison for the class of Michèle Sebag. Along similar line, F. Landes proposed a challenge in the context of S. Mallat’s course, at Collège de France. Finally, in collaboration with aiforgood.org, and Heri Rakotoarison has put in place a hackathon for the conference Data Science Africa (https://codalab.lri.fr/competitions/522)

[0] https://indico.cern.ch/event/813759/

In terms of dissemination, four books were published in 2019 in the Springer series on challenges in machine learning, see http://www.chalearn.org/books.html.

CQFD Project-Team

6. New Results

6.1. Power-of-d-Choices with Memory: Fluid Limit and Optimality

Abstract: In multi-server distributed queueing systems, the access of stochastically arriving jobs to resources is often regulated by a dispatcher, also known as load balancer. A fundamental problem consists indesigning a load balancing algorithm that minimizes the delays experienced by jobs. During the last twodecades, the power-of-d-choice algorithm, based on the idea of dispatching each job to the least loadedserver out ofdservers randomly sampled at the arrival of the job itself, has emerged as a breakthroughin the foundations of this area due to its versatility and appealing asymptotic properties. In this paper,we consider the power-of-d-choice algorithm with the addition of a local memory that keeps track of thelatest observations collected over time on the sampled servers. Then, each job is sent to a server withthe lowest observation. We show that this algorithm is asymptotically optimal in the sense that the load balancer can always assign each job to an idle server in the large-system limit. Our results quantify and highlight the importance of using memory as a means to enhance performance in randomized load balancing.

Authors: J. Anselmi (CQFD); F. Dufour (CQFD).

6.2. Hamilton-Jacobi-Bellman Inequality for the Average Control of Piecewise Deterministic Markov Processes

Abstract : The main goal of this work is to study the infinite-horizon long run average continuous-time optimal control problem of piecewise deterministic Markov processes (PDMPs) with the control acting continuously on the jump intensity λ and on the transition measure Q of the process.

Authors : O.L.V. Costa; F. Dufour (CQFD)

6.3. Approximation of discounted minimax Markov control problems and zero-sum Markov games using Hausdorff and Wasserstein distances

Abstract : This work 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 μ. 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 : F. Dufour (CQFD); T. Prieto-Rumeau

6.4. Combining clustering of variables and feature selection using random forests: the CoV/VSURF procedure

Abstract : Standard approaches to tackle high-dimensional supervised classification problem often include variable selection and dimension reduction procedures. The novel methodology proposed in this paper combines clustering of variables and feature selection. More precisely, hierarchical clustering of variables procedure allows to build groups of correlated variables in order to reduce the redundancy of information and summarizes each group by a synthetic numerical variable. Originality is that the groups of variables (and the number of groups) are unknown a priori. Moreover the clustering approach used can deal with both numerical and categorical variables (i.e. mixed dataset). Among all the possible partitions resulting from dendrogram cuts, the most relevant synthetic variables (i.e. groups of variables) are selected with a variable selection procedure using random forests. Numerical performances of the proposed approach are compared with direct applications of random forests and variable selection using random forests on the original p variables. Improvements obtained with the proposed methodology are illustrated on two simulated mixed datasets (cases $n>p$ and $n<p$, where n is the sample size) and on a real proteomic dataset. Via the selection of groups of variables (based on the synthetic variables), interpretability of the results becomes easier.

Authors : Marie Chavent (CQFD), Robin Genuer (SISTM), Jerome Saracco (CQFD)

6.5. Statistical model choice including variable selection based on variable importance: A relevant way for biomarkers selection to predict meat tenderness

Abstract : In this work, we describe a new computational methodology to select the best regression model to predict a numerical variable of interest Y and to select simultaneously the most interesting numerical explanatory variables strongly linked to Y. Three regression models (parametric, semi-parametric and non-parametric) are considered and estimated by multiple linear regression, sliced inverse regression and random forests. Both the variables selection and the model choice are computational. A measure of importance based on random perturbations is calculated for each covariate. The variables above a threshold are selected. Then a learning/test samples approach is used to estimate the Mean Square Error and to determine which model (including variable selection) is the most accurate. The R package modvarsel (MODel and VARiable SELection) implements this computational approach and applies to any regression datasets. After checking the good behavior of the methodology on simulated data, the R package is used to select the proteins predictive of meat tenderness among a pool of 21 candidate proteins assayed in semitendinosus muscle from 71 young bulls. The biomarkers were selected by linear regression (the best regression model) to predict meat tenderness. These biomarkers, we confirm the predominant role of heat shock proteins and metabolic ones.

Authors : Marie-Pierre Ellies-Oury, Marie Chavent, Alexandre Conanec, Jérôme Saracco

6.6. Genome sequencing for rightward hemispheric language dominance

Abstract : Most people have left-hemisphere dominance for various aspects of language processing, but only roughly 1 % of the adult population has atypically reversed, rightward hemispheric language dominance (RHLD). The genetic-developmental program that underlies leftward language laterality is unknown, as are the causes of atypical variation. We performed an exploratory whole-genome-sequencing study, with the hypothesis that strongly penetrant, rare genetic mutations might sometimes be involved in RHLD. This was by analogy with situs inversus of the visceral organs (left-right mirror reversal of the heart, lungs etc.), which is sometimes due to monogenic mutations. The genomes of 33 subjects with RHLD were sequenced, and analysed with reference to large population-genetic datasets, as well as thirty-four subjects (14 left-handed) with typical language laterality. The sample was powered to detect rare, highly penetrant, monogenic effects if they would be present in at least 10 of the 33 RHLD cases and no controls, but no individual genes had mutations in more than 5 RHLD cases while being un-mutated in controls. A hypothesis derived from invertebrate mechanisms of left-right axis formation led to the detection of an increased mutation load, in

RHLD subjects, within genes involved with the actin cytoskeleton. The latter finding offers a first, tentative insight into molecular genetic influences on hemispheric language dominance.

Authors : Amaia Carrion-castillo, Lise van der Haegen, Nathalie Tzourio-mazoyer, Tulya Kavaklioglu, Solveig Badillo, Marie Chavent, Jérôme Saracco, Marc Brysbaert, Simon Fisher, Bernard Mazoyer, Clyde Francks

6.7. An Original Methodology for the Selection of Biomarkers of Tenderness in Five Different Muscles

Abstract : For several years, studies conducted for discovering tenderness biomarkers have proposed a list of 20 candidates. The aim of the present work was to develop an innovative methodology to select the most predictive among this list. The relative abundance of the proteins was evaluated on five muscles of 10 Holstein cows: gluteobiceps, semimembranosus, semitendinosus, Triceps brachii and Vastus lateralis. To select the most predictive biomarkers, a multi-block model was used: The Data-Driven Sparse Partial Least Square. Semimembranosus and Vastus lateralis muscles tenderness could be well predicted (R^2= 0.95 and 0.94 respectively) with a total of 7 out of the 5 times 20 biomarkers analyzed. An original result is that the predictive proteins were the same for these two muscles: μ-calpain, m-calpain, h2afx and Hsp40 measured in m. gluteobiceps and μ-calpain, m-calpain and Hsp70-8 measured in m. Triceps brachii. Thus, this method is well adapted to this set of data, making it possible to propose robust candidate biomarkers of tenderness that need to be validated on a larger population.

Authors : Ellies-Oury, M.-P., Lorenzo, H., Denoyelle, C., Conanec, A., Saracco, J., Picard B.

6.8. New Approach Studying Interactions Regarding Trade-Off between Beef Performances and Meat Qualities

Abstract : The beef cattle industry is facing multiple problems, from the unequal distribution of added value to the poor matching of its product with fast-changing demand. Therefore, the aim of this study was to examine the interactions between the main variables, evaluating the nutritional and organoleptic properties of meat and cattle performances, including carcass properties, to assess a new method of managing the trade-off between these four performance goals. For this purpose, each variable evaluating the parameters of interest has been statistically modeled and based on data collected on 30 Blonde d'Aquitaine heifers. The variables were obtained after a statistical pre-treatment (clustering of variables) to reduce the redundancy of the 62 initial variables. The sensitivity analysis evaluated the importance of each independent variable in the models, and a graphical approach completed the analysis of the relationships between the variables. Then, the models were used to generate virtual animals and study the relationships between the nutritional and organoleptic quality. No apparent link between the nutritional and organoleptic properties of meat (r = -0.17) was established, indicating that no important trade-off between these two qualities was needed. The 30 best and worst profiles were selected based on nutritional and organoleptic expectations set by a group of experts from the INRA (French National Institute for Agricultural Research) and Institut de l'Elevage (French Livestock Institute). The comparison between the two extreme profiles showed that heavier and fatter carcasses led to low nutritional and organoleptic quality.

Authors : Conanec ,A., Picard, B., Cantalapiedra-Hijar, G., Chavent, M., Denoyelle, C., Gruffat, D., Normand, J., Saracco, J., Ellies-Oury M.P.

6.9. Impact of Speller Size on a Visual P300 Brain-Computer Interface (BCI) System under Two Conditions of Constraint for Eye Movement

Abstract : The vast majority of P300-based brain-computer interface (BCI) systems are based on the well-known P300 speller presented by Farwell and Donchin for communication purposes and an alternative to people with neuromuscular disabilities, such as impaired eye movement. The purpose of the present work is to study the effect of speller size on P300-based BCI usability, measured in terms of effectiveness, efficiency, and

satisfaction under overt and covert attention conditions. To this end, twelve participants used three speller sizes under both attentional conditions to spell 12 symbols. The results indicated that the speller size had, in both attentional conditions, a significant influence on performance. In both conditions (covert and overt), the best performances were obtained with the small and medium speller sizes, both being the most effective. The speller size did not significantly affect workload on the three speller sizes. In contrast, covert attention condition produced very high workload due to the increased resources expended to complete the task. Regarding users' preferences, significant differences were obtained between speller sizes. The small speller size was considered as the most complex, the most stressful, the less comfortable, and the most tiring. The medium speller size was always considered in the medium rank, which is the speller size that was evaluated less frequently and, for each dimension, the worst one. In this sense, the medium and the large speller sizes were considered as the most satisfactory. Finally, the medium speller size was the one to which the three standard dimensions were collected: high effectiveness, high efficiency, and high satisfaction. This work demonstrates that the speller size is an important parameter to consider in improving the usability of P300 BCI for communication purposes. The obtained results showed that using the proposed medium speller size, performance and satisfaction could be improved.

Authors :Ron-Angevin, R., Garcia, L., Fernandez-Rodriguez, A., Saracco, J., André, J.-M., Lespinet-Najib, V.

6.10. High-Dimensional Multi-Block Analysis of Factors Associated with Thrombin Generation Potential

Abstract : The identification of novel biological factors associated with thrombin generation, a key biomarker of the coagulation process, remains a relevant strategy to disentangle pathophysiological mechanisms underlying the risk of venous thrombosis (VT). As part of the MARseille THrombosis Association Study (MARTHA), we measured whole blood DNA methylation levels, plasma levels of 300 proteins, 3 thrombin generation biomarkers (endogeneous thrombin potential, peak and lagtime), clinical and genetic data in 700 patients with VT. The application of a novel high-dimensional multi-levels statistical methodology we recently developed, the data driven sparse Partial Least Square method (ddsPLS), on the MARTHA datasets enabled us 1/ to confirm the role of a known mutation of the variability of endogenous thrombin potential and peak, 2/ to identify a new signature of 7 proteins strongly associated with lagtime.

Authors : Lorenzo, H., Razzaq, M., Odeberg, J., Saracco, J., Tregouet, D.-A., Thiébaut, R.

6.11. Multiple-output quantile regression through optimal quantization

Abstract : A new nonparametric quantile regression method based on the concept of optimal quantization was developed recently and was showed to provide estimators that often dominate their classical, kernel-type, competitors. In the present work, we extend this method to multiple-output regression problems. We show how quantization allows approximating population multiple-output regression quantiles based on halfspace depth. We prove that this approximation becomes arbitrarily accurate as the size of the quantization grid goes to infinity. We also derive a weak consistency result for a sample version of the proposed regression quantiles. Through simulations, we compare the performances of our estimators with (local constant and local bilinear) kernel competitors. The results reveal that the proposed quantization-based estimators, which are local constant in nature, outperform their kernel counterparts and even often dominate their local bilinear kernel competitors. The various approaches are also compared on artificial and real data.

Authors : Charlier, I., Paindaveine, D., Saracco, J.

6.12. Artificial evolution, fractal analysis and applications

Abstract :

This document contains a selection of research works to which I have contributed. It is structured around two themes, artificial evolution and signal regularity analysis and consists of three main parts: Part I: Artificial evolution, Part II: Estimation of signal regularity and Part III: Applications, combination of signal processing, fractal analysis and artificial evolution. In order to set the context and explain the coherence of the rest of the document, this manuscript begins with an introduction, Chapter 1, providing a list of collaborators and of the research projects carried out. Theoretical contributions focus on two areas: evolutionary algorithms and the measurement of signal regularity and are presented in Part I and Part II respectively. These two themes are then exploited and applied to real problems in Part III. Part I, Artificial Evolution, consists of 8 chapters. Chapter 2 contains a brief presentation of various types of evolutionary algorithms (genetic algorithms, evolutionary strategies and genetic programming) and presents some contributions in this area, which will be detailed later in the document. Chapter 3, entitled Prediction of Expected Performance for a Genetic Programming Classifier proposes a method to predict the expected performance for a genetic programming (GP) classifier without having to run the program or sample potential solutions in the research space. For a given classification problem, a pre-processing step to simplify the feature extraction process is proposed. Then the step of extracting the characteristics of the problem is performed. Finally, a PEP (prediction of expected performance) model is used, which takes the characteristics of the problem as input and produces the predicted classification error on the test set as output. To build the PEP model, a supervised learning method with a GP is used. Then, to refine this work, an approach using several PEP models is developed, each now becoming a specialized predictors of expected performance (SPEP) specialized for a particular group of problems. It appears that the PEP and SPEP models were able to accurately predict the performance of a GP-classifier and that the SPEP approach gave the best results. Chapter 4, entitled A comparison of fitness-case sampling methods for genetic programming presents an extensive comparative study of four fitness-case sampling methods, namely: Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and the proposed Keep-Worst Interleaved Sampling. The algorithms are compared on 11 symbolic regression problems and 11 supervised classification problems, using 10 synthetic benchmarks and 12 real-world datasets. They are evaluated based on test performance, overfitting and average program size, comparing them with a standard GP search. The experimental results suggest that fitness-case sampling methods are particularly useful for difficult real-world symbolic regression problems, improving performance, reducing overfitting and limiting code growth. On the other hand, it seems that fitness-case sampling cannot improve upon GP performance when considering supervised binary classification. Chapter 5, entitled Evolving Genetic Programming Classifiers with Novelty Search, deals with a new and unique approach towards search and optimization, the Novelty Search (NS), where an explicit objective function is replaced by a measure of solution novelty. This chapter proposes a NS-based GP algorithm for supervised classification. Results show that NS can solve real-world classification tasks, the algorithm is validated on real-world benchmarks for binary and multiclass problems. Moreover, two new versions of the NS algorithm are proposed, Probabilistic NS (PNS) and a variant of Minimal Criteria NS (MCNS). The former models the behavior of each solution as a random vector and eliminates all of the original NS parameters while reducing the computational overhead of the NS algorithm. The latter uses a standard objective function to constrain and bias the search towards high performance solutions. This chapter also discusses the effects of NS on GP search dynamics and code growth. The results show that NS can be used as a realistic alternative for supervised classification, and specifically for binary problems the NS algorithm exhibits an implicit bloat control ability. In Chapter 6, entitled Evaluating the Effects of Local Search in Genetic Programming, a memetic GP that incorporates a local search (LS) strategy to refine GP individuals expressed as syntax trees is studied in the context of symbolic regression. A simple parametrization for GP trees is proposed, by weighting each function with a parameter (unique for each function used in the construction of a tree). These parameters are then optimized using a trust region optimization algorithm which is therefore used here as a local search method. Then different heuristic methods are tested over several benchmark and real-world problems to determine which individuals from the tree population should be subjected to a LS. The results show that the best performances (in term of both quality of the solution and bloat control) was achieved when LS is applied to all of the solutions or to random individuals chosen from the top percentile (with respect to fitness) of the population. Chapter 7, entitled A Local Search Approach to Genetic Programming for Binary Classification, proposes a memetic GP, tailored for binary classification problems, extending the work on symbolic regression presented in the previous chapter. In particular, a small linear subtree is added on the top of the root node of the original tree and each node in a tree is weighted by a real-valued parameter, which is then numerically optimized using the trust-region algorithm used as a local search method. Experimental results show that potential classifiers produced by GP are improved by the local searcher, and hence the overall search is improved achieving substantial performance gains. Application on well-known benchmarks provided results competitive with state-of-the-art. Chapter 8, entitled RANSAC-GP: Dealing with Outliers in Symbolic Regression with Genetic Programming, presents a hybrid methodology based on the RAndom SAmpling Consensus (RANSAC) algorithm and GP, called RANSAC-GP. RANSAC is an approach to deal with outliers in parameter estimation problems, widely used in computer vision and related fields. This work presents the first application of RANSAC to symbolic regression with GP. The proposed algorithm is able to deal with extreme amounts of contamination in the training set, evolving highly accurate models even when the amount of outliers reaches 90Part II, Estimation of signal regularity consists of 3 chapters. Chapter 9, entitled Hölderian Regularity, provides some reminders and some theoretical contributions on the estimation of Hölderian regularity. Some details are given on the estimation of the Hölder exponent using oscillation method or a wavelet transform. These approaches and improved versions are compared on synthetic signals. The FracLab software, were all the above methods have been integrated, is also presented at the end of this chapter. The work proposed in Chapter 10, entitled Theoretical comparison of the DFA and variants for the estimation of the Hurst exponent, involves a theoretical and numerical comparison between the Detrended Fluctuation Analysis (DFA) and its variants, namely DMA, AFA, RDFA and the proposed Continuous DFA method, in which the trend is constrained to be continuous. The DFA is a well-established method to detect long-range correlations in time series. It has been used in a wide range of applications, from biomedical applications to signal denoising. It allows the Hurst exponent of a pure mono-fractal time series to be estimated. It operates as follows: after integration, the signal is split into segments. Using a least-squares criterion, local trends are deduced. The resulting piecewise linear trend is then subtracted to the whole signal. The power of the residual is computed for different segment lengths and its log-log representation allows the Hurst exponent to be deduced. The comparison performed in this chapter is based on a new common matrix writing formalism of the square of the fluctuation function from the instantaneous correlation function of the process for all these methods. In the case where the process under study is stationary in the broad sense, the statistical mean of the square of the fluctuation function is thus expressed as a weighted sum of the terms of the autocorrelation function, and this without any approximation. More precisely, the mathematical expectation of the square of the fluctuation function can be seen for each method as the autocorrelation function of the output of a filter dependent on this method and calculated for a lag equal to zero, i.e. the power of the filter output. In the general case, this analytical framework provides a means of comparing the DFA and its variants that is different from a traditional synthetic signal performance study, and explains the different behaviours of these regularity estimation methods, using the proposed filter analysis. Chapter 11 contains two patents with THALES AVS related to the work presented in the previous chapter. Part III of this manuscript, Applications, combination of signal processing, fractal analysis and artificial evolution, contains contributions combining the tools previously mentioned in order to develop new tools such as in the Chapters 12 and 13 or contributions on the resolution of real problems in the biomedical field, such as in the Chapters 14, 15 and 16. Chapter 12, entitled "The Estimation of Hölderian Regularity using Genetic Programming", presents a GP approach to synthesize estimators for the pointwise Hölder exponent in 2D signals. The optimization problem to solve is to minimize the error between a prescribed regularity and the estimated regularity given by an image operator. The search for optimal estimators is then carried out using a GP algorithm. Experiments confirm that the GPoperators produce a good estimation of the Hölder exponent in images of multifractional Brownian motions. In fact, the evolved estimators significantly outperform a traditional method by as much as one order of magnitude. These results provide further empirical evidence that GP can solve difficult problems of applied mathematics. In Chapter 13, entitled "Optimization of the Hölder Image Descriptor using a Genetic Algorithm", a local descriptor based on the Hölder exponent is studied. The proposal is to find an optimal number of dimensions for the descriptor using a genetic algorithm (GA). To guide the GA search, fitness is computed based on the performance of the descriptor when applied to standard region matching problems. This criterion is quantified using the F-Measure, derived from recall and precision analysis. Results show that it is possible to reduce the size of the canonical Hölder descriptor without degrading the quality of its performance. In fact, the best descriptor found through the GA search is nearly 70performance on standard tests. Chapter 14, entitled "Interactive evolution for cochlear implants fitting", presents a study that intends to make cochlear implants more adaptable to environment and to simplify the process of fitting, by designing and using a specific interactive evolutionary algorithm combined with signal processing. Real experiments on volunteer implanted patients are presented, that show the efficiency of interactive evolution for this purpose. In Chapter 15, entitled "Feature extraction and classification of EEG signals. The use of a genetic algorithm for an application on alertness prediction", the development of computer systems for the automatic analysis and classification of mental states of vigilance; i.e., a person's state of alertness is studied. Such a task is relevant to diverse domains, where a person is expected or required to be in a particular state. For instance, pilots, security personnel or medical staffs are expected to be in a highly alert state, and a brain computer interface could help confirm this or detect possible problems. In this chapter, a combination of an evolutionary algorithm and signal processing is used. The purpose of this algorithm was to select an electrode and a frequency range to use in order to discriminate between the two states of vigilance. This approach determined the most useful electrode for the classification task. Using the recording of this electrode, the prediction obtained has a reliability rate of 89.33

In Chapter 16, entitled "Regularity and Matching Pursuit Feature Extraction for the Detection of Epileptic Seizures", a novel methodology for feature extraction on EEG signals that allows to perform a highly accurate classification of epileptic states is presented. Specifically, Hölderian regularity and the Matching Pursuit algorithm are used as the main feature extraction techniques, and are combined with basic statistical features to construct the final feature sets. These sets are then delivered to a Random Forests classification algorithm to differentiate between epileptic and non-epileptic readings. Several versions of the basic problem are tested and statistically validated producing perfect accuracy in most problems and 97.6a well known database, reveals that the proposal achieves state-of-the-art performance.The experimental results suggest that using a feature extraction methodology composed of regularity analysis, a Matching Pursuit algorithm and time-domain statistic measures together with a classifier produces a system that can predict epileptic states with competitive performance that matches or even surpass other novel methods. Finally the last chapter concludes this manuscript and provides perspectives for future work.

Authors : Pierrick Legrand

6.13. Self-affinity of an Aircraft Pilot's Gaze Direction as a Marker of Visual Tunneling

Abstract : For the last few years, a great deal of interest has been paid to crew monitoring systems in order to tackle potential safety problems during a flight. They aim at detecting any degraded physiological and/or cognitive state of an aircraft pilot, such as attentional tunneling or excessive focalization. Indeed, they might have a negative impact on his performance to pursue his mission with adequate flight safety levels. One of the usual approaches consists in using sensors to collect physiological signals which are analyzed in real-time. Two main families exist to process the signals. The first one combines feature extraction and machine learning whereas the second is based on deep-learning approaches but may require a large amount of labelled data. Here, we focused on the first family. In this case, various features can be deduced from the data by different approaches: spectrum analysis, a priori modelling and nonlinear dynamical system analysis techniques including the estimation of the self-affinity of the signals. In this paper, our purpose was to analyze whether the self-affinity of the pilot gaze direction can be related to his cognitive state. To this end, an experiment was carried out on 18 subjects in a representative aircraft environment based on a modified version of the software MATB-II. The scenarii were designed to elicit different levels of mental workload eventually associated to attentional tunneling. A database to train the machine learning step was first created by recording the directions of gaze of the subjects with an eye-tracker. The self-affinities of these signals were extracted with the Detrended Fluctuation Analysis method. They constituted the inputs of the classifier based on a Support Vector Machine. Then, new signals were analyzed and classified. Preliminary results showed promising abilities to detect attentional tunnelling episodes for different levels of mental workload.

Authors : Bastien Berthelot, Patrick Mazoyer, Sarah Egea, Jean-Marc André, Eric Grivel

6.14. Filtering-based Analysis Comparing the DFA with the CDFA for Wide Sense Stationary Processes

Abstract : The detrended fluctuation analysis (DFA) is widely used to estimate the Hurst exponent. Although it can be outperformed by wavelet based approaches, it remains popular because it does not require a strong expertise in signal processing. Recently, some studies were dedicated to its theoretical analysis and its limits. More particularly, some authors focused on the so-called fluctuation function by searching a relation with an estimation of the normalized covariance function under some assumptions. This paper is complementary to these works. We first show that the square of the fluctuation function can be expressed in a similar matrix form for the DFA and the variant we propose, called Continuous-DFA (CDFA), where the global trend is constrained to be continuous. Then, using the above representation for wide-sense-stationary processes, the statistical mean of the square of the fluctuation function can be expressed from the correlation function of the signal and consequently from its power spectral density, without any approximation. The differences between both methods can be highlighted. It also confirms that they can be seen as ad hoc wavelet based techniques.

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Jean-Marc André, Patrick Mazoyer, et al

6.15. 2D Fourier Transform Based Analysis Comparing the DFA with the DMA

Abstract : Even if they can be outperformed by other methods, the detrended fluctuation analysis (DFA) and the detrended moving average (DMA) are widely used to estimate the Hurst exponent because they are based on basic notions of signal processing. For the last years, a great deal of interest has been paid to compare them and to better understand their behaviors from a mathematical point of view. In this paper, our contribution is the following: we first propose to express the square of the socalled fluctuation function as a 2D Fourier transform (2D-FT) of the product of two matrices. The first one is defined from the instantaneous correlations of the signal while the second, called the weighting matrix, is representative of each method. Therefore, the 2D-FT of the weighting matrix is analyzed in each case. In this study, differences between the DFA and the DMA are pointed out when the approaches are applied on non-stationary processes

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Marc Donias, Jean-Marc André, et al.

6.16. Interpréter les Fonctions de Fluctuation du DFA et du DMA comme le Résultat d'un Filtrage

Abstract : The detrended uctuation analysis (DFA) and the detrending moving average (DMA) are often used to estimate the regularity of the signal, since they do not require a strong expertise in the eld of signal processing while providing good results. In this paper, our contribution is twofold. We propose a framework that allows these approaches to be compared. It is based on a matrix form of the square of the uctuation function. Using the above representation for wide-sense-stationary processes, we show that the statistical mean of the square of the uctuation function can be expressed from the correlation function of the signal and consequently from its power spectral density, without any approximation. The dierences between both methods can be highlighted. It also conrms that they can be seen as ad hoc wavelet based techniques to estimate the Hurst exponent.

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Jean-Marc Andre, Patrick Mazoyer, et al.

6.17. A perturbation analysis of stochastic matrix Riccati diffusions

Abstract : Matrix differential Riccati equations are central in filtering and optimal control theory. The purpose of this article is to develop a perturbation theory for a class of stochastic matrix Riccati diffusions. Diffusions of this type arise, for example, in the analysis of ensemble Kalman-Bucy filters since they describe the flow of certain sample covariance estimates. In this context, the random perturbations come from the fluctuations of a mean field particle interpretation of a class of nonlinear diffusions equipped with an interacting sample covariance matrix functional. The main purpose of this article is to derive non-asymptotic

Taylor-type expansions of stochastic matrix Riccati flows with respect to some perturbation parameter. These expansions rely on an original combination of stochastic differential analysis and nonlinear semigroup techniques on matrix spaces. The results here quantify the fluctuation of the stochastic flow around the limiting deterministic Riccati equation, at any order. The convergence of the interacting sample covariance matrices to the deterministic Riccati flow is proven as the number of particles tends to infinity. Also presented are refined moment estimates and sharp bias and variance estimates. These expansions are also used to deduce a functional central limit theorem at the level of the diffusion process in matrix spaces.

Authors : Adrian N. Bishop, Pierre Del Moral, Angele Niclas

6.18. On the stability of matrix-valued Riccati diffusions

Abstract : The stability properties of matrix-valued Riccati diffusions are investigated. The matrix-valued Riccati diffusion processes considered in this work are of interest in their own right, as a rather prototypical model of a matrix-valued quadratic stochastic process. Under rather natural observability and controllability conditions, we derive time-uniform moment and fluctuation estimates and exponential contraction inequalities. Our approach combines spectral theory with nonlinear semigroup methods and stochastic matrix calculus. This analysis seem to be the first of its kind for this class of matrix-valued stochastic differential equation. This class of stochastic models arise in signal processing and data assimilation, and more particularly in ensemble Kalman-Bucy filtering theory. In this context, the Riccati diffusion represents the flow of the sample covariance matrices associated with McKean-Vlasov-type interacting Kalman-Bucy filters. The analysis developed here applies to filtering problems with unstable signals.

Authors : Adrian N. Bishop, Pierre Del Moral

6.19. A variational approach to nonlinear and interacting diffusions

Abstract : The article presents a novel variational calculus to analyze the stability and the propagation of chaos properties of nonlinear and interacting diffusions. This differential methodology combines gradient flow estimates with backward stochastic interpolations, Lyapunov linearization techniques as well as spectral theory. This framework applies to a large class of stochastic models including non homogeneous diffusions, as well as stochastic processes evolving on differentiable manifolds, such as constraint-type embedded manifolds on Euclidian spaces and manifolds equipped with some Riemannian metric. We derive uniform as well as almost sure exponential contraction inequalities at the level of the nonlinear diffusion flow, yielding what seems to be the first result of this type for this class of models. Uniform propagation of chaos properties w.r.t. the time parameter are also provided. Illustrations are provided in the context of a class of gradient flow diffusions arising in fluid mechanics and granular media literature. The extended versions of these nonlinear Langevin-type diffusions on Riemannian manifolds are also discussed.

Authors : Marc Arnaudon (IMB), Pierre Del Moral (CMAP, CQFD)

6.20. An explicit Floquet-type representation of Riccati aperiodic exponential semigroups

Abstract : The article presents a rather surprising Floquet-type representation of time-varying transition matrices associated with a class of nonlinear matrix differential Riccati equations. The main difference with conventional Floquet theory comes from the fact that the underlying flow of the solution matrix is aperiodic. The monodromy matrix associated with this Floquet representation coincides with the exponential (fundamental) matrix associated with the stabilizing fixed point of the Riccati equation. The second part of this article is dedicated to the application of this representation to the stability of matrix differential Riccati equations. We provide refined global and local contraction inequalities for the Riccati exponential semigroup that depend linearly on the spectral norm of the initial condition. These refinements improve upon existing results and are a direct consequence of the Floquet-type representation, yielding what seems to be the first results of this type for this class of models.

Authors : Adrian N. Bishop, Pierre Del Moral

6.21. Uniform propagation of chaos and creation of chaos for a class of nonlinear diffusions

Abstract : We are interested in nonlinear diffusions in which the own law intervenes in the drift. This kind of diffusions corresponds to the hydrodynamical limit of some particle system. One also talks about propagation of chaos. It is well-known, for McKean-Vlasov diffusions, that such a propagation of chaos holds on finite-time interval. We here aim to establish a uniform propagation of chaos even if the external force is not convex, with a diffusion coefficient sufficiently large. The idea consists in combining the propagation of chaos on a finite-time interval with a functional inequality, already used by Bolley, Gentil and Guillin, see [BGG12a, BGG12b]. Here, we also deal with a case in which the system at time t = 0 is not chaotic and we show under easily checked assumptions that the system becomes chaotic as the number of particles goes to infinity together with the time. This yields the first result of this type for mean field particle diffusion models as far as we know.

Authors : Pierre Del Moral and Julian Tugaut

6.22. Stability Properties of Systems of Linear Stochastic Differential Equations with Random Coefficients

Abstract : This work is concerned with the stability properties of linear stochastic differential equations with random (drift and diffusion) coefficient matrices, and the stability of a corresponding random transition matrix (or exponential semigroup). We consider a class of random matrix drift coefficients that involves random perturbations of an exponentially stable flow of deterministic (time-varying) drift matrices. In contrast with more conventional studies, our analysis is not based on the existence of Lyapunov functions, and it does not rely on any ergodic properties. These approaches are often difficult to apply in practice when the drift/diffusion coefficients are random. We present rather weak and easily checked perturbation-type conditions for the asymptotic stability of time-varying and random linear stochastic differential equations. We provide new log-Lyapunov estimates and exponential contraction inequalities on any time horizon as soon as the fluctuation parameter is sufficiently small. These seem to be the first results of this type for this class of linear stochastic differential equations with random coefficient matrices.

Authors : Adrian N. Bishop, Pierre Del Moral

6.23. On One-Dimensional Riccati Diffusions

Abstract : This article is concerned with the fluctuation analysis and the stability properties of a class of one-dimensional Riccati diffusions. These one-dimensional stochastic differential equations exhibit a quadratic drift function and a non-Lipschitz continuous diffusion function. We present a novel approach, combining tangent process techniques, Feynman-Kac path integration, and exponential change of measures, to derive sharp exponential decays to equilibrium. We also provide uniform estimates with respect to the time horizon, quantifying with some precision the fluctuations of these diffusions around a limiting deterministic Riccati differential equation. These results provide a stronger and almost sure version of the conventional central limit theorem. We illustrate these results in the context of ensemble Kalman-Bucy filtering. To the best of our knowledge, the exponential stability and the fluctuation analysis developed in this work are the first results of this kind for this class of nonlinear diffusions.

Authors: Adrian N. Bishop, Pierre Del Moral, Kengo Kamatani, Bruno Remillard

6.24. Adaptive Approximate Bayesian Computational Particle Filters for Underwater Terrain-Aided Navigation.

Authors : C. Palmier, K. Dahia, N. Merlinge, P. Del Moral, D. Laneuville & C. Musso

6.25. Inference for conditioned Galton-Watson trees from their Harris path

Tree-structured data naturally appear in various fields, particularly in biology where plants and blood vessels may be described by trees, but also in computer science because XML documents form a tree structure. This paper is devoted to the estimation of the relative scale parameter of conditioned GaltonWatson trees. New estimators are introduced and their consistency is stated. A comparison is made with an existing approach of the literature. A simulation study shows the good behavior of our procedure on finite-sample sizes and from missing or noisy data. An application to the analysis of revisions of Wikipedia articles is also considered through real data.

Authors: Romain Azaïs, Alexandre Genadot and Benoit Henry

MATHRISK Project-Team

7. New Results

7.1. Control of systemic risk in a dynamic framework

Agnès Sulem, Andreea Minca (Cornell University), Hamed Amini (J. Mack Robinson College of Business, Georgia State University) and Rui Chen have studied a Dynamic Contagion Risk Model With Recovery Features [27]. In this paper, they introduce threshold growth in the classical threshold contagion model, in which nodes have downward jumps when there is a failure of a neighboring node. Choosing the configuration model as underlying graph, they prove fluid limits for the baseline model, as well as extensions to the directed case, state-dependent inter-arrival times and the case of growth driven by upward jumps. They obtain explicit ruin probabilities for the nodes according to their characteristics: initial threshold and in- (and out-) degree. They then allow nodes to choose their connectivity by trading off link benefits and contagion risk. They define a rational equilibrium concept in which nodes choose their connectivity according to an expected failure probability of any given link, and then impose condition that the expected failure probability coincides with the actual failure probability under the optimal connectivity. Existence of an asymptotic equilibrium is shown as well as convergence of the sequence of equilibria on the finite networks. In particular, these results show that systems with higher overall growth may have higher failure probability in equilibrium.

The results have been presented in Lisbon at the COMPLEX NETWORKS 2019 conference. Rui Chen has defended his thesis in July 2019 on this topic [10].

7.2. Mean-field BSDEs and systemic risk measures

Agnès Sulem with her PhD student Rui Chen, Andreea Minca and Roxana Dumitrescu have studied mean-field BSDEs with a generalized mean-field operator that can capture the average intensity in an inhomogeneous random graph. Comparison and strict comparison results have been obtained. Based on these, they interpret the BSDE solution as a global dynamic risk measure that can account for the intensity of system interactions and therefore incorporate systemic risk. Using Fenchel-Legendre transforms, they establish a dual representation for the expectation of the risk measure, and exhibit its dependence on the mean-field operator [31].

7.3. Risk management in finance and insurance

7.3.1. Option pricing in a non-linear incomplete market model with default

Agnès Sulem has studied with Miryana Grigorova (University of Leeds) and Marie-Claire Quenez (Université Paris Denis Diderot) superhedging prices and the associated superhedging strategies for both European and American options (see [33] and [32] in a non-linear incomplete market model with default. The underlying market model consists of a risk-free asset and a risky asset driven by a Brownian motion and a compensated default martingale. The portfolio processes follow non-linear dynamics with a non-linear driver f.

7.3.2. Neural network regression for Bermudan option pricing

The pricing of Bermudan options amounts to solving a dynamic programming principle, in which the main difficulty, especially in high dimension, comes from the conditional expectation involved in the computation of the continuation value. These conditional expectations are classically computed by regression techniques on a finite dimensional vector space. In [36], Bernard Lapeyre and Jérôme Lelong study neural networks approximations of conditional expectations. They prove the convergence of the well-known Longstaff and Schwartz algorithm when the standard least-square regression is replaced by a neural network approximation. They illustrate the numerical efficiency of neural networks as an alternative to standard regression methods for approximating conditional expectations on several numerical examples.

7.3.3. Hybrid numerical method for option pricing

With Giulia Terenzi, Lucia Caramellino (Tor Vegata University), and Maya Briani (CNR Roma), Antonino Zanette develop and study stability properties of a hybrid approximation of functionals of the Bates jump model with stochastic interest rate that uses a tree method in the direction of the volatility and the interest rate and a finite-difference approach in order to handle the underlying asset price process. They also propose hybrid simulations for the model, following a binomial tree in the direction of both the volatility and the interest rate, and a space-continuous approximation for the underlying asset price process coming from a Euler–Maruyama type scheme. They test their numerical schemes by computing European and American option prices [17].

7.3.4. American options

With his PhD student Giulia Terenzi, Damien Lamberton has been working on American options in Heston's model [22]. He is currently preparing his contribution to a winter school on "Theory and practice of optimal stopping and free boundary problems" (cf. https://conferences.leeds.ac.uk/osfbp/).

7.3.5. Solvency Capital Requirement 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.

A. Alfonsi and his PhD student A. Cherchali have developed a model of the ALM management of insurance companies that takes into account the regulatory constraints on life-insurance [25]. We now focus on developing Multilevel Monte-Carlo methods to approximate the SCR (Solvency Capital Requirement).

7.3.6. Pricing and hedging variable annuities of GMWB type in advanced stochastic models

Antonino Zanette with Ludovic Goudenège (Ecole Centrale de Paris) and Andrea Molent (University of Udine) study the valuation of a particular type of variable annuity called GMWB when advanced stochastic models are considered. As remarked by Yang and Dai (Insur Math Econ 52(2):231–242, 2013), and Dai et al. (Insur Math Econ 64:364–379, 2015), the Black–Scholes framework seems to be inappropriate for such a long maturity products. Also Chen et al. (Insur Math Econ 43(1):165–173, 2008) show that the price of GMWB variable annuities is very sensitive to the interest rate and the volatility parameters. They propose here to use a stochastic volatility model (the Heston model) and a Black–Scholes model with stochastic interest rate (the Black–Scholes Hull–White model). For this purpose, they consider four numerical methods: a hybrid tree-finite difference method, a hybrid tree-Monte Carlo method, an ADI finite difference scheme and a Standard Monte Carlo method. These approaches are employed to determine the no-arbitrage fee for a popular version of the GMWB contract and to calculate the Greeks used in hedging. Both constant withdrawal and dynamic withdrawal strategies are considered. Numerical results are presented, which demonstrate the sensitivity of the no-arbitrage fee to economic and contractual assumptions as well as the different features of the proposed numerical methods [18].

7.4. Stochastic Analysis and probabilistic numerical methods

7.4.1. Particles approximation of mean-field SDEs

O. Bencheikh and Benjamin Jourdain analysed the rate of convergence of a system of N interacting particles with mean-field rank based interaction in the drift coefficient and constant diffusion coefficient [16], [30]. They first adapted arguments by Kolli and Shkolnikhov to check trajectorial propagation of chaos with optimal rate

$N^{-1/2}$ to the associated stochastic differential equations nonlinear in the sense of McKean. They next relaxed the assumption needed by Bossy to check convergence in $L^1(\mathbf{R})$ of the empirical cumulative distribution function of the Euler discretization with step h of the particle system to the solution of a one dimensional viscous scalar conservation law with rate $\mathcal{O}\left(\frac{1}{\sqrt{N}}+h\right)$. Last, they proved that the bias of this stochastic particle method behaves in $\mathcal{O}\left(\frac{1}{N}+h\right)$, which is confirmed by numerical experiments.

7.4.2. Abstract Malliavin calculus and convergence in total variation

In collaboration with L. Caramellino (University Tor Vergata) and with G. Poly (University of Rennes), V. Bally has settled a Malliavin type calculus for a general class of random variables, which are not supposed to be Gaussian (as it is the case in the standard Malliavin calculus). This is an alternative to the Γ calculus settled by Bakry, Gentile and Ledoux. The main application is the estimate in total variation distance of the error in general convergence theorems. This is done in [29].

7.4.3. Invariance principles

As an application of the methodology mentioned above, V. Bally and coauthors have studied several limit theorems of Central Limit type - (see [14] and [15]. In particular they have estimate the total variation distance between random polynomials on one hand, and proved an universality principle for the variance of the number of roots of trigonometric polynomials with random coefficients, on the other hand.

7.4.4. Regularity of the low of the solution of jump type equations

V. Bally, L. Caramellino and G. Poly obtained some new regularity results for the solution of the 2 dimensional Bolzmann equation (see [13]). Moreover, in collaboration with L. Caramellino and A. Kohatsu Higa, V. Bally has started a research program on the regularity of the solutions of jump type equations. A first result in this sense is contained in [28].

7.4.5. Approximation of ARCH models

Benjamin Jourdain and Gilles Pagès (LPSM) are interested in proposing approximations of a sequence of probability measures in the convex order by finitely supported probability measures still in the convex order [35]. They propose to alternate transitions according to a martingale Markov kernel mapping a probability measure in the sequence to the next and dual quantization steps. In the case of ARCH models and in particular of the Euler scheme of a driftless Brownian diffusion, the noise has to be truncated to enable the dual quantization step. They analyze the error between the original ARCH model and its approximation with truncated noise and exhibit conditions under which the latter is dominated by the former in the convex order at the level of sample-paths. Last, they analyse the error of the scheme combining the dual quantization steps with truncation of the noise according to primal quantization.

7.4.6. Convergence of metadynamics

By drawing a parallel between metadynamics and self interacting models for polymers, B. Jourdain, T. Lelièvre (Cermics / ENPC) and P.-A. Zitt (LAMA) study the longtime convergence of the original metadynamics algorithm in the adiabatic setting, namely when the dynamics along the collective variables decouples from the dynamics along the other degrees of freedom. They also discuss the bias which is introduced when the adiabatic assumption does not holds [34].

7.4.7. Optimal transport

With V. Ehrlacher, D. Lombardi and R. Coyaud, Aurelien Alfonsi isworking on numerical a approximations of the optimal transport between two (or more) probability measures [26].

7.4.8. Generic approximation schemes for Markov semigroups.

A. Alfonsi and V. Bally have produced a general approximation scheme for Markov semigroups, based on random grids. This is a new approach to approximation schemes which is an alternative to the multi level method and the Romberg method [24].

7.4.9. Approximation with rough paths

A. Alfonsi and A. Kebaier are working on the approximation of some processes with rough paths.

SIMSMART Project-Team

5. New Results

5.1. Objective 1 – Rare events simulation

In [2], 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 [1], 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. In [1] we extend the central limit theorem to the case of synchronized branchings, where re-sampling of particles is performed after any given number of particles have been killed. The result is obtained in the generic case of Fleming-Viot particle systems.

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 [5], 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.

In [24], we consider Langevin processes, which are widely used in molecular simulation to compute reaction kinetics using rare event algorithms. We prove convergence in distribution in the overdamped asymptotics. The proof relies on the classical perturbed test function (or corrector) method, which is used both to show tightness in path space, and to identify the extracted limit with a martingale problem. The result holds assuming the continuity of the gradient of the potential energy, and a mild control of the initial kinetic energy.

5.2. Objective 2 – High dimensional filtering

The work presented in [10] is about solutions for 2D multitarget tracking from image observations including its application on radar data and results on simulated data. Tracking from image observations rather than from detected points is often referred to as track–before–detect (TBD). The objective is to capture targets with a low signal–to–noise ratio (SNR) which would not be detected or tracked after data thresholding. The highly nonlinear filtering equations are approximated using a particle filter implementation. This nonlinearity emerges from the observation function which relies on the radar treatment chain, involving matched filtering of a chirp signal, and beamforming achieved from a linear phased array, leading to the raw data image. Amplitudes and phases of target–returned signals are considered as temporally fluctuating, random and unknown, creating non–deterministic contributions of the targets to the signal to deal with.

5.3. Objective 3 – Non-paramatric statistics

Production forecast errors are the main hurdle to integrate variable renewable energies into electrical power systems. Regardless of the technique, these errors are inherent in the forecast exercise, although their magnitude significantly vary depending on the method and the horizon. As power systems have to balance out these errors, their dynamic and stochastic modeling is valuable for the real time operation. The study in [23] proposes a Markov Switching Auto Regressive – MS-AR – approach. After having validated its statistical relevance, this model is used to solve the problem of the optimal management of a storage associated with a wind power plant when this virtual power plant must respect a production commitment.

5.4. Objective 4 – Model Reduction

Model reduction aims at proposing efficient algorithmic procedures for the resolution (to some reasonable accuracy) of high-dimensional systems of parametric equations. This overall objective entails many different subtasks:

1) the identification of low-dimensional surrogates of the target “solution” manifold 2) The devise of efficient methodologies of resolution exploiting low-dimensional surrogates 3) The theoretical validation of the accuracy achievable by the proposed procedures

This year, we made several contributions to these subtasks. In most of our contributions, we deviated from the standard working hypothesis involving a linear subspace surrogate.

In a first group of publications, we concentrated our attention on the so-called “sparse” low-dimensional model. In this context, we have proposed several new algorithmic solutions to decrease the computational complexity associated to projection onto this low-dimensional model. These methodologies take place in the context of “screening” procedures for LASSO. We first introduced a new screening strategy, dubbed "joint screening test", which allows the rejection of a set of atoms by performing one single test, see [4]. Our approach enables to find good compromises between complexity of implementation and effectiveness of screening. Second, we proposed 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, see [11]. We finally showed in another work that the main concepts underlying screening procedures can be extended to different families of convex optimization problems, see [22].

Another avenue of research has been the study of the sparse surrogate in the context of “continuous” dictionaries, where the elementary signals forming the decomposition catalog are functions of some parameters taking its values in some continuously-valued domain. In this context, we contributed to the theoretical characterization of the performance of some well-known algorithmic procedure, namely “orthogonal matching pursuit” (OMP). More specifically, we proposed the first theoretical analysis of the behavior of OMP in the continuous setup, see [12], [17], [21]. We also provided a new connection between two popular low-rank approximations of continuous dictionaries, namely the “polar” and “SVD” approximations, see [9].

The tools exploited in the field of model-order reduction and sparsity have found some particular applicative field in geophysics and fluid mechanics. In [8], [7], we derived procedures based on sparse representations to localize the positions of particles in a moving fluid. In [16], [15], [14], [26], [27], we designed learning methodologies to learn the dynamical model underlying a set of observed data.

5.5. Miscellaneous

In [25], 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.

In [6], we consider the problem of predicting a categorical variable based on groups of inputs. Some methods have already been proposed to elaborate classifi- cation rules based on groups of variables (e.g. group lasso for logistic regression). However, to our knowledge, no tree-based approach has been proposed to tackle this issue. Here, we propose the Tree Penalized Linear Discriminant Analysis algorithm (TPLDA), a new-tree based approach which constructs a classification rule based on groups of variables.

TOSCA Team

6. New Results

6.1. Probabilistic numerical methods, stochastic modeling and applications

Participants: Sofia Allende Contador, Alexis Anagnostakis, Mireille Bossy, Lorenzo Campana, Nicolas Champagnat, Quentin Cormier, Madalina Deaconu, Aurore Dupre, Coralie Fritsch, Vincent Hass, Pascal Helson, Christophe Henry, Ulysse Herbach, Igor Honore, Antoine Lejay, Rodolphe Loubaton, Radu Maftei, Kerlyns Martinez Rodriguez, Victor Martin Lac, Hector Olivero-Quinteros, Édouard Strickler, Denis Talay, Etienne Tanré, Denis Villemonais.

6.1.1. Published works and preprints

- H. AlRachid (Orléans University), M. Bossy, C. Ricci (University of Florence) and L. Szpruch (University of Edinburgh and The Alan Turing Institute, London) introduced several new particle representations for *ergodic* McKean-Vlasov SDEs. They construct new algorithms by leveraging recent progress in weak convergence analysis of interacting particle system. In [12] they present detailed analysis of errors and associated costs of various estimators, highlighting key differences between long-time simulations of linear (classical SDEs) versus non-linear (McKean-Vlasov SDEs) process.
- 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 (LEMON team) obtained advances in stochastic Lagrangian approaches for the simulation of hydrokinetic turbines immersed in complex topography [42].
- M. Bossy, J.-F. Jabir (University of Edinburgh) and K. Martinez (University of Valparaiso) consider the problem of the approximation of the solution of a one-dimensional SDE with non-globally Lipschitz drift and diffusion coefficients behaving as x^{α}, with $\alpha > 1$ [44]. They propose an (semi-explicit) exponential-Euler scheme and study its convergence through its weak approximation error. To this aim, they analyze the $C^{1,4}$ regularity of the solution of the associated backward Kolmogorov PDE using its Feynman-Kac representation and the flow derivative of the involved processes. From this, under some suitable hypotheses on the parameters of the model ensuring the control of its positive moments, they recover a rate of weak convergence of order one for the proposed exponential Euler scheme. Numerical experiments are analyzed in order to complement their theoretical result.
- L. Campana et al. developed some Lagrangian stochastic model for anisotropic particles in turbulent flow [35]. Suspension of anisotropic particles can be found in various industrial applications. Microscopic ellipsoidal bodies suspended in a turbulent fluid flow rotate in response to the velocity gradient of the flow. Understanding their orientation is important since it can affect the optical or rheological properties of the suspension (e.g. polymeric fluids). The equations of motion for the orientation of microscopic ellipsoidal particles was obtained by Jeffery. But so far this description has been always investigated in the framework of direct numerical simulations (DNS) and experimental measurements. In this work, the orientation dynamics of rod-like tracer particles, i.e. long ellipsoidal particles (in the limit of infinite aspect-ratio) is studied. The size of the rod is assumed smaller than the Kolmogorov length scale but sufficiently large that its Brownian motion need not be considered. As a result, the local flow around a particle can be considered as inertia-free and Stokes flow solutions can be used to relate particle rotational dynamics to the local velocity gradient. The orientation of rod can be described as the normalised solution of the linear ordinary differential equation for the separation vector between two fluid tracers, under the action of the velocity gradient tensor. In this framework, the rod orientation is described by a Lagrangian stochastic model where cumulative velocity gradient fluctuations are represented by a white-noise tensor such that the incompressibility condition is preserved. A numerical scheme based on the decomposition into skew/symmetric part of the process dynamics is proposed.

- 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 [13].
- Together with M. Benaïm (Univ, Neuchâtel), N. Champagnat and D. Villemonais studied stochastic algorithms to approximate quasi-stationary distributions of diffusion processes absorbed at the boundary of a bounded domain. They study a reinforced version of the diffusion, which is resampled according to its occupation measure when it reaches the boundary. They show that its occupation measure converges to the unique quasi-stationary distribution of the diffusion process [43].
- N. Champagnat, C. Fritsch and S. Billiard (Univ. Lille) studied models of food web adaptive evolution. They identified the biomass conversion efficiency as a key mechanism underlying food webs evolution and discussed the relevance of such models to study the evolution of food webs [51].
- N. Champagnat and J. Claisse (Univ. Paris-Dauphine) 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 [18].
- 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 [19].
- 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 distributions of the Fleming-Viot processes approach a particular QSD, called minimal QSD. They proved that this holds true for general absorbed Markov processes with soft obstacles [20].
- N. Champagnat and D. Villemonais studied the geometric convergence of normalized unbounded semigroups. They proved in [47] that general criteria for this convergence can be easily deduced from their recent results on the theory of quasi-stationary distributions.
- N. Champagnat, S. Méléard (École Polytechnique) and V.C. Tran (Univ. Paris Est Marne-la-Vallée) studied evolutionary models of bacteria with horizontal transfer. They considered in [46] a scaling of parameters taking into account the influence of negligible but non-extinct populations, allowing them to study specific phenomena observed in these models (re-emergence of traits, cyclic evolutionary dynamics and evolutionary suicide).
- M. Bahlali (CEREA, France) , C. Henry and B. Carissimo (CEREA, France) clarify issues related to the expression of Lagrangian stochastic models used for atmospheric dispersion applications. They showed that accurate simulations are possible only if two aspects are properly addressed: the respect of the well-mixed criterion (related to the incorporation of the mean pressure-gradient term in the mean drift-term) and the consistency between Eulerian and Lagrangian turbulence models (regarding turbulence models, boundary and divergence-free conditions).
- A. Lejay and A. Brault have continued their work on rough flows, which provides an unified framework to deal with the theory of rough paths from the point of view of flows. In particular, they have studied consistency, stability and generic properties of rough differential equations [45].
- A. Lejay and P. Pigato have provided an estimator of a discontinuous drift coefficients [30], which follows their previous work on the oscillating Brownian motion and its application to financial models.

- A. Lejay and H. Mardones (U. la Serenan, Chile), have completed their work on the Monte Carlo simulation of the Navier-Stockes equations based on a new representation by Forward-Backward Stochastic Differential Equations [53].
- O. Faugeras, E. Soret and E. Tanré have obtained a Mean-Field description of thermodynamics limits of large population of neurons with random interactions. They have obtained the asymptotic behaviour for an asymmetric neuronal dynamics in a network of linear Hopfield neurons. They have a complete description of this limit with Gaussian processes. Furthermore, the limit object is not a Markov process [50].
- 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 [24].
- P. Helson has studied the learning of an external signal by a neural network and the time to forget it when this network is submitted to noise. He has constructed an estimator of the initial signal thanks to the synaptic currents, which are Markov chains. The mathematical study of the Markov chains allow to obtain a lower bound on the number of external stimuli that the network can receive before the initial signal is forgotten [52].
- 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 Volterra equation satisfied by this rate. They used methods from integral equation to control finely the long time behavior of this firing rate [21].
- 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 $n \to \infty$ [23].
- O. Faugeras, James Maclaurin (Univ. of Utah) and E. Tanré have worked on the asymptotic behavior of a model of neurons in interaction with correlated gaussian synaptic weights. They have obtained the limit equation as a singular non-linear SDE and a Large Deviation Principle for the law of the finite network [49].
- E. Tanré has worked with Alexandre Richard (Centrale-Supelec) and Soledad Torres (Universidad de Valparaíso, Chile) on a one-dimensional fractional SDE with reflection. They have proved the existence of the reflected SDE with a penalization scheme (suited to numerical approximation). Penalization also gives an algorithm to approach this solution [55].
- The Neutron Transport Equation (NTE) describes the flux of neutrons over time through an inhomogeneous fissile medium. A probabilistic solution of the NTE is considered in order to demonstrate a Perron-Frobenius type growth of the solution via its projection onto an associated leading eigenfunction. The associated eigenvalue, denoted k_{eff}, has the physical interpretation as being the ratio of neutrons produced (during fission events) to the number lost (due to absorption in the reactor or leakage at the boundary) per typical fission event. Together with A. M. G. Cox, E. L. Horton and A. E. Kyprianou (Univ. Bath), D. Villemonais developed the stochastic analysis of the NTE by giving a rigorous probabilistic interpretation of k_{eff} [48].

- In [34], D. Villemonais obtained a lower bound for the coarse Ricci curvature of continuous-time pure-jump Markov processes, with an emphasis on interacting particle systems. Applications to several models are provided, with a detailed study of the herd behavior of a simple model of interacting agents.
- In collaboration with C. Coron (Univ. Paris Sud) and S. Méléard (École Polytechnique), D. Villemonais studied in [22] the way alleles extinctions and fixations occur for a multiple allelic proportions model based on diffusion processes. It is proved in particular that alleles extinctions occur successively and that a 0-1 law holds for fixation and extinction: depending on the population dynamics near extinction, either fixation occurs before extinction, or the converse, almost surely.
- Mean telomere length in human leukocyte DNA samples reflects the different lengths of telomeres at the ends of the 23 chromosomes and in an admixture of cells. Together with S. Toupance (CHRU Nancy), D. Germain (Univ. Lorraine), A. Gégout-Petit (Univ. Lorraine and BIGS Inria team), E. Albuisson (CHRU Nancy) and A. Benetos (CHRU Nancy), D. Villemonais analysed telomere length distributions dynamics in adults individuals. It is proved in [33] that the shape of this distribution is stable over the lifetime of individuals.
- J. Bion-Nadal (Ecole Polytechnique) and D. Talay have pursued their work on their 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 [15].

  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, approximations of the optimal model have been established. The construction and analysis of an efficient stochastic algorithm are being in progress.
- D. Talay and M. Tomašević have continued to work on their new type of stochastic interpretation of the 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. D. Talay and M. Tomašević are studying the well-posedness and the propagation of chaos of the particle system related to the two-dimensional parabolic-parabolic Keller-Segel system.
- V. Martin Lac, R. Maftei D. Talay and M. Tomašević have continued to work on theoretical and algorithmic questions related to the simulation of the Keller–Segel particle systems. The library DIAMSS has been developed.
- H. Olivero (Inria, now University of Valparaiso, Chile) and D. Talay have continued to work on their 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.
- I. Honoré and D. Talay have worked on statistical issues related to numerical approximations of invariant probability measures of ergodic diffusions. These approximations are based on the simulation of one single trajectory up to long time horizons. I. Honoré and D. Talay handle the critical situations where the asymptotic variance of the normalized error is infinite.
- 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 have ended the second volume of their series on Mathematical Foundation of Stochastic Simulation to be published by Springer.

6.1.2. Other works in progress

- K. Martinez, M. Bossy, C. Henry, R. Maftei and S. Sherkarforush work on a refined algorithm for macroscopic simulations of particle agglomeration using population balance equations (PBE). More precisely, their study is focused on identifying regions with non-homogeneous spatial distribution of particles. This is indeed a major drawback of PBE formulations which require a well-mixed condition to be satisfied. The developed algorithm identifies higher/lower density regions to treat them separately.
- S. Allende (CEMEF, France), J. Bec (CEMEF, France), M. Bossy, L. Campana, M. Ferrand (EDF, France), C. Henry and J.P. Minier (EDF, France) work together on a macroscopic model for the dynamics of small, flexible, inextensible fibers in a turbulent flow. Following the model developed at Inria, they perform numerical simulations of the orientation of such fibers in wall-bounded turbulent flows and compare it to microscopic simulations obtained with Direct Numerical Simulation (DNS). This work is performed under the POPART project.
- N. Champagnat, C. Fritsch and U. Herbach are working with A. Harlé (Institut de Cancérologie de Lorraine), J.-L. Merlin (ICL), E. Pencreac'h (CHRU Strasbourg), A. Gégout-Petit, P. Vallois, A. Muller-Gueudin (Inria BIGS team) and A. Kurtzmann (Univ. Lorraine) within an ITMO Cancer project on modeling and parametric estimation of dynamical models of circulating tumor DNA (ctDNA) of tumor cells, divided into several clonal populations. The goal of the project is to predict the emergence of a clonal population resistant to a targeted therapy in a patient's tumor, so that the therapy can be modulated more efficiently.
- N. Champagnat and R. Loubaton are working with P. Vallois (Univ. Lorraine and Inria BIGS team) and L. Vallat (CHRU Strasbourg) on the inference of dynamical gene networks from RNAseq and proteome data.
- N. Champagnat, E. Strickler and D. Villemonais are working on the characterization of convergence in Wasserstein distance of conditional distributions of absorbed Markov processes to a quasi-stationary distribution.
- N. Champagnat and V. Hass are studying evolutionary models of adaptive dynamics under an assumption of large population and small mutations. They expect to recover variants of the canonical equation of adaptive dynamics, which describes the long time evolution of the dominant phenotype in the population, under less stringent biological assumptions than in previous works.
- Q. Cormier, E. Tanré and Romain Veltz (team MATHNEURO) are working on the local stability of a stationary solution of some McKean-Vlasov equation. They also obtain spontaneous oscillation of the solution for critical values of the external currents or the interactions.
- M. Deaconu, A. Lejay and E. Mordecki (U. de la República, Uruguay) are studying an optimal stopping problem for the Snapping Out Brownian motion.
- M. Deaconu and A. Lejay are currently working on the simulation and the estimation of the fragmentation equation through its probabilistic representation.
- S. Allende (CEMEF, France) , C. Henry and J. Bec (CEMEF, France) work on the dynamics of small, flexible, inextensible fibers in a turbulent flow. They show that the fragmentation of fibers smaller than the smallest fluid scale in a turbulent flow occurs through tensile fracture (i.e. when the fiber is stretched along its main axis) or through flexural failure (i.e. when the fiber curvature is too high as it buckles under compressive load). Statistics of such events are provide together with measures of the rate of fragmentation and daughter size distributions, which are basic ingredients for macroscopic fragmentation models.

- C. Henry and M.L. Pedrotti (LOV, France) are working together on the topic of sedimentation of plastic that are populated by biological organisms (this is called biofouling). Biofouling modifies the density of plastic debris in the ocean and can lead to their sedimentation towards deeper regions. This work is done under the PLAISE project, which comprises measurements (by the LOV) and simulations (by C. Henry).
- 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.
- C. Fritsch is working with Tanjona Ramiadantsoa (Univ. Wisconsin-Madison) on a model of extinction of orphaned plants.
- A. Lejay and M. Clausel (U. Lorraine) are studing the clustering method based on the use of the signature and the iterated integrals of time series. It is based on asymmetric spectral clustering [41].
- In collaboration with L. Lenotre (postdoc at IECL between Oct. 2018 and Sep. 2019), A. Gégout-Petit (Univ. Lorraine and Inria BIGS team) and O. Coudray (Master degree student), D. Villemonais conducted preliminary researches on branching models for the telomeres' length dynamics across generations.